Accuracy of topological entanglement entropy on finite cylinders

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Topological phases are unique states of matter which support non-local excitations which behave as particles with fractional statistics. A universal characterization of gapped topological phases is provided by the topological entanglement entropy (TEE). We study the finite size corrections to the TEE by focusing on systems with $Z_2$ topological ordered state using density-matrix renormalization group (DMRG) and perturbative series expansions. We find that extrapolations of the TEE based on the Renyi entropies with Renyi index $n \geq 2$ suffer from much larger finite size corrections than do extrapolations based on the von Neumann entropy. In particular, when the circumference of the cylinder is about ten times the correlation length, the TEE obtained using von Neumann entropy has an error of order $10^{-3}$, while for Renyi entropies it can even exceed 40%. We discuss the relevance of these findings to previous and future searches for topological ordered phases, including quantum spin liquids.

The work above utilized the von Neumann entanglement entropy, and achieved an accurate extrapolation of the TEE term. In the literature, many works study instead the generalized Renyi entropies, defined as

$$S_n(A) = \frac{1}{1-n} \ln \text{Tr} \rho_A^n,$$

while the von Neumann entropy $S_1$ is defined as the limit $n \to 1$. For simplicity, we will call $S_n$ as Renyi entanglement entropy when $n \geq 2$, while von Neumann entanglement entropy when $n = 1$. Theoretically, the universal TEE is expected to obtain also for the Renyi entropy, with $\gamma$ independent of the Renyi index. However, extrapolations in the literature based on the Renyi entropy appear to be substantially less accurate than those based on the von Neumann entropy, even for larger boundary lengths $L$.

In this letter, we study the finite-size effects in the TEE systematically for two canonical models of phases with $Z_2$ topological order, and confirm the above suggestion. We attempt to cast our results in terms of the expected form,

$$S_n(L) = \alpha_n L - \gamma_n,$$

as a function of Renyi index $n$. First, we study the Toric-Code model whose TEE is known, using DMRG and perturbative series expansions. We then turn to the more realistic $S = 1/2$ antiferromagnetic Heisenberg model on the Kagome lattice. For both cases, we find that the Renyi entropies do have substantially larger finite-size corrections than the von Neumann entropy. We provide some understanding of this tendency from the fact, which we show from the series expansion, that the line term $\alpha_n$...
FIG. 1: (Color online) The extrapolated TEE $\gamma_n$ using von Neumann entropy (i.e., $n = 1$) and Renyi entropy (i.e., $n \geq 2$) for the Toric-Code model, as a function of the applied magnetic field $h_x$, for (a) $h_z = 0$ and (b) symmetric case $h_z = h_x$. The dashed lines represent the expected universal value, $\ln 2$, for the TEE in the thermodynamic limit.

FIG. 2: (Color online) Moving two point data fits for the extrapolated TEE $\gamma_n$ for the Toric-Code model for (a) $h_x = 0.3$ with $h_z = 0$, and (b) $h_x = h_z = 0.3$, as a function of the cylinder circumference $L_y$ and entropy index $n$. Here, $\gamma_n(L_y)$ are fitted using two data points, i.e., $S_n(L_y)$ and $S_n(L_y + 2)$ using Eq. (1). The dashed lines represent the expected asymptotic value $\gamma = \ln 2$.
not aware of any exact perturbative evaluation of its line entropy relevant to our geometry. In order to carry out this calculation, we turn to Linked Cluster Methods.\[13\]

We consider one of the ground state sectors of the TCM and map the problem on to the Transverse-Field Ising Model (TFIM) if only $h_x$ is non-zero\[14\] and on to a $\mathbb{Z}_2$ Lattice-gauge model if both $h_x$ and $h_z$ are non-zero.\[16\] In either case, one has a unique non-degenerate ground state. Here, we will consider only the former mapping and the case with only $h_x$ non-zero. Up to 4-th order, the dependence on $h_x$ and $h_z$ are additive and hence knowing the dependence on $h_x$ and the symmetry under the interchange of $h_x$ and $h_z$ one can easily write down the full dependence on $h_x$ and $h_z$.

Given the exact mapping between the models, if we were to calculate some property like the ground state energy in a series expansion in the field, the expansions would be identical to the TFIM. However, there is a crucial difference for the entanglement entropies.\[20\] The TFIM variables sit at the center of the plaquettes whereas the TCM variables and the perturbing fields live on the bonds. Furthermore, each state in the TCM is a linear superposition of many basis states (say in the $\sigma_z$ basis). This affects how the states are represented on either side of the partition and hence the reduced density matrix as we discuss below.

In the linked cluster method, we can define a cluster by a set of bonds, where the perturbative fields are present.\[21, 22\] The entanglement entropies can be expressed as

$$S_n = \sum_c W_n(c),$$

(2)

where $S_n$ is the entanglement entropy in any model, where there are those clusters that are (i) linked and (ii) that contain at least one bond in subsystem A and one in subsystem B.\[21, 22\] Here, one should note that two bonds are linked if they meet at a site or if they are on the opposite sides of an elementary plaquette (because they can both change the flux through a common plaquette). This implies that all such clusters must be situated close to the interface between A and B. Since such linked clusters can be translated along the line, it follows that, for a large system, this entropy is proportional to the length of the line. In fourth order, we can group the perturbations into just two distinct clusters, whose calculational details can be found in the Supplementary materials.

For line term of the Renyi entropy for $n > 1$, to order $h^4$, we obtain

$$\alpha_n = \frac{1}{2} \left( \ln 2 - \frac{n}{32} h^4 + \frac{3n}{n-1} \frac{h^4}{128} \right)$$

(4)

while, the von-Neumann entropy ($n \to 1$) becomes

$$\alpha_1 = \frac{1}{2} \left( \ln 2 - \left( \frac{33}{128} - \frac{5}{32} \ln 2 \right) h^4 - \frac{3}{32} h^4 \ln h \right).$$

(5)

Note that the innocuous $h^n \ln h$ singularity is inevitable for the von-Neumann entropy in any model, where there are Schmidt states, whose weight is zero in the unperturbed model but becomes non-zero as a power of the perturbation parameter.

In Fig.\[20\] we show the line entropies $\alpha_n$ obtained in DMRG compared with the series expansion results (See also Fig.\[3\] in Supplementary materials). The agreement is excellent. The important thing to note is the $n$ dependence of the line entropy. The linear $n$ dependence in Eq.\[4\] means that with increasing $n$, the line entropy changes more rapidly with the applied fields. Since, the topological entanglement entropy is obtained after subtraction of the much larger line entropy, it follows that with increasing $n$ the entanglement entropy would have a much larger finite size correction, as the correlation length increases.

**Kagome Heisenberg Model** We now turn to the spin-1/2 Heisenberg model on the Kagome lattice, for which compelling\[23, 24\] and direct evidence\[9, 12\] for a $\mathbb{Z}_2$ topological quantum spin liquid has been obtained by extensive DMRG studies. In particular, highly accurate TEE $\gamma_1 = \ln(2)$ has been obtained using cylinder construction\[9, 12\], for the model with both first- and

FIG. 3: (Color online) Line entropy $\alpha_n$ obtained from DMRG (block square) and perturbative calculation (red circle) for both von Neumann entropy (i.e., $n = 1$) and Renyi entropy (i.e., $n \geq 2$) for the Toric-Code model, as a function of the magnetic field $h_x$, here $h_x = 0$. 

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second-neighbor interactions – see the Supplementary Information for details of the definition. Specifically, the extrapolated TEE $\gamma_n$ for the Kagome $J_1$-$J_2$ Heisenberg model as a function of entropy index $n$ at both $J_2 = 0.10$ and $J_2 = 0.15$. Inset: $\gamma_n$ for TCM as a function of entropy index $n$, for the case $h_x = 0.3, h_z = 0.3$ (black square), and the symmetric case $h_x = h_z = 0.3$ (red circle). The dashed lines correspond to $\ln(2)$.

As in the TCM, we find that the Renyi entropies give much less accurate estimates of $\gamma_n$. The extrapolated TEE $\gamma_n$ for $n \geq 2$ clearly deviates from the expected value, even when the cylinder circumference is much larger than the correlation length, i.e., $L_y \approx 10\xi$ (the correlation lengths are known from the earlier study in Ref.[9]). For example, as shown in Fig. 3, a linear fit using Eq. 1 gives $\gamma_2 \approx 0.42(1)$ at both $J_2 = 0.10$ and $J_2 = 0.15$: a huge error of $\sim 40\%$. Moreover, with increasing Renyi index $n$, the deviation becomes even larger, reaching, for example $\sim 60\%$ for $n = 4$, as shown in Fig. 4. These results show that large finite-size corrections to the Renyi entropies obtain not only in the “artificial” TCM, but also in realistic quantum spin Hamiltonians.

**Summary and Conclusion** In this paper, we studied the finite-size scaling of the TEE for systems with $Z_2$ topological order, using DMRG simulations and perturbative series expansions. We find that generally the finite-size errors in the TEE based on the Renyi entropy estimators (i.e., $n \geq 2$) are much larger than those obtained from the von Neumann entropy (i.e., $n = 1$). In particular, when the cylinder circumference is around ten times the correlation length, $L_y \approx 10\xi$, the extrapolated TEE using von Neumann entropy is quite accurate with an error of order $10^{-3}$. On the contrary, the error can be orders of magnitude larger for Renyi entropy. For instance, for spin-1/2 Kagome Heisenberg model, the error is only around a fraction of percent for von Neumann entropy, while it is 40% or even larger for Renyi entropy. Perturbative study of the TCM shows that the larger finite-size corrections for the TEE originates in part from the enhanced variation with parameters of the line entropy $\alpha_n$ with increasing $n$. This indicates moreover that estimates of the TEE become less accurate with increasing $n$. We note that errors of the magnitude found here for $n \geq 2$ in the Kagome Heisenberg model are large enough to perhaps preclude a definitive identification of the topological phase, even if we assume that a universal value obtains in the thermodynamic limit. Our results clearly indicate that great care must be taken into account for finite size corrections in numerical calculations of the TEE, particularly those based on Renyi entropies with $n \geq 2$. This gives techniques, such as DMRG, which have direct access to the full density matrix and hence von Neumann entropy, a distinct advantage. Although in this paper we have focused on systems with $Z_2$ topological order, similar conclusions may be expected more generally.

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Supplementary Information

I. Toric-Code Model in Magnetic Field

The Toric-Code model[1] with an applied magnetic field is given by

\[ H = -J_s \sum_s A_s - J_p \sum_p B_p - h_z \sum_i \sigma_i^z - h_x \sum_i \sigma_i^x (S1) \]

where \( \sigma_i^x \) and \( \sigma_i^z \) are Pauli matrices, \( A_s = \Pi_{i\in s} \sigma_i^x \) and \( B_p = \Pi_{i\in p} \sigma_i^z \). Subscripts \( s \) and \( p \) refer respectively to vertices and plaquettes on the square lattice, whereas \( i \) runs over all bonds where spin degrees of freedom are located. Without magnetic field, i.e., \( h_x = h_z = 0 \), the pure TCM can be solved exactly[1]. It exhibits a 4-fold ground state degeneracy on the torus, and has \( Z_2 \) topological order with total quantum dimension \( D = 2 \). All elementary excitations are gapped and characterized by eigenvalues \( A_s = -1 \) (a \( Z_2 \) charge on site \( s \)) and \( B_p = -1 \) (a \( Z_2 \) vortex on plaquette \( p \)). After turning on the magnetic fields, the model cannot be solved exactly anymore. However, previous studies[14–16] show that the \( Z_2 \) topological phase remains quite stable and robust until the magnetic fields are large enough to induce a phase transition from the topological phase to the trivial one. Specifically, such a phase transition takes place at the critical magnetic field \( h_x^c \approx 0.32 \) when \( h_z = 0 \), while \( h_x^c \approx 0.34 \) along the symmetric line with \( h_z = h_x \).

For the DMRG simulation, we consider an equivalent square lattice, where the spin operators \( \sigma^x \) and \( \sigma^z \) sit on the sites instead of the bonds. Therefore, the star operator \( A_s \) and the plaquette operator \( B_p \) of the original lattice now sit on alternating plaquettes in the equivalent square lattice, as shown in Figure S1, labeled as \( S \) and \( P \), respectively. Note that on this equivalent square lattice, there are an even number of dangling spins within each plaquette at the open edges. For the pure Toric-Code model with cylinder boundary condition, the first \( 2^{L_y/2-1} \) eigenvalues of the reduced density matrix \( \rho_A \) are degenerate and equal to \( 1/2^{L_y/2-1} \), while all the other eigenvalues are zero. Therefore, the entanglement entropy, defined as \( S_n = -\frac{1}{n-1} \ln \text{Tr} \rho_A^n \), does not depend on the entropy index \( n \), and is equal to \( S_n = \frac{\ln(2)}{2} L_y - \ln(2) \), with coefficient \( \alpha_n = \ln(2)/2 \) and TEE \( \gamma_n = \ln(2) \).

After turning on the magnetic field, the degeneracy of entanglement spectrum is lifted, and the correlation length \( \xi \) becomes finite, as shown in Figure S2 (note that other types of the correlation length may be defined, but are expected to differ just by a factor of order 1 from the above one). Therefore, the entanglement entropy \( S_n \) will depend on the entropy index \( n \), and it follows that
so too will the coefficient $\alpha_n$ and the extrapolated TEE $\gamma_n$. Indeed, our results show that when approaching the phase transition point (e.g., $h_x = 0.34$ along the symmetric line with $h_x = h_z$), the dependence of the TEE $\gamma_n$ on $n$ becomes clearer and clearer, as shown in Fig.1(b) in the main text, and Fig.S1 here. For example, the correlation length $\xi \approx 1$ lattice spacing at $h_x^c = 0.3$, and the resulting TEE $\gamma_1 = 0.696(4)$ obtained from the von Neumann entanglement entropy is still quite accurate with an error around a few fraction of $10^{-3}$, i.e., $\sim 0.4\%$. On the contrary, the fitted TEE $\gamma_n$ using Renyi entropy (i.e., $n \geq 2$) deviates from the expected value clearly, with an error more than order of magnitude larger than for $\gamma_1$. For instance, $\gamma_2 = 0.726(6)$, with an error around 5%, around one order of magnitude larger than that for $\gamma_1$. Such a deviation is even larger with the increase of $n$, e.g., $\gamma_4 = 0.762(8)$, with an error around 10%, more than one order of magnitude larger than that for $\gamma_1$.

Deviations are also found in the line entropies $\alpha_n$. Fig.S3 shows the comparison for $\alpha_n$ obtained numerically using Eq.1 and theoretically using Eq.4 up to 4th order series expansion. The series expansion results match the DMRG values remarkably accurately, though as expected, the difference between the two increases markedly on approaching the phase transition point, especially for larger $n$.

**II. Perturbative calculations**

The perturbative calculations to order $h^4$ for the Toric Code Model require just two clusters shown in Fig.S4 (i) A cluster consisting of all four bonds incident on a boundary site between A and B and (ii) A cluster with two bonds across a plaquette facing each other across the boundary between A and B. The first has a count of one per boundary site. The second has a count of 2 per boundary site. Once grouped this way, no subgraph subtraction is needed in 4th order.

We now discuss the calculation of $S_n(c)$, the Renyi entropy when only the fields on the bonds of a cluster $c$ are present.[22] First the ground state wavefunction is calculated perturbatively in the TFIM variables, with all the perturbing fields present in the cluster. Then, for every basis state in the TFIM model, a representative $\sigma_z$ basis state is obtained in the TCM variable. When all the 4 perturbative fields are present at a site, the states in the TCM must be enlarged by the operation of the projection operator $1 + A_s$ at the site. This will give us the ground state for the cluster in the TCM variables. Once, the ground state for the cluster is known in the TCM variables, it is straightforward to calculate the reduced density matrix for subsystem $A$ and hence the entanglement entropies, $S_n(c)$.

First we consider graph (ii) from the figure. This graph has just two bonds, one in $A$ and one in $B$. In the lan-

![FIG. S4: Graphs needed for the perturbative calculation of the line entropy to 4th order. The dashed line separates subsystems A and B. The solid lines denote the perturbing fields in the cluster.](image)
guage of TFIM, there are three plaquettes on which Visons can be created or destroyed. However, since Visons are created or destroyed in pairs, there are only 4 relevant states in the Hilbert space. These can be denoted by the number of Visons present in the plaquette as $|1\rangle = |0,0,0\rangle$, $|2\rangle = |1,1,0\rangle$, $|3\rangle = |0,1,1\rangle$ and $|4\rangle = |1,0,1\rangle$. These four states can be related to the TCM in terms of $\sigma_z$ on the two bonds of the cluster. The four states become $|1\rangle = |1,1\rangle$, $|2\rangle = |-1,1\rangle$, $|3\rangle = |1,-1\rangle$ and $|4\rangle = |-1,-1\rangle$. In this 4-dimensional Hilbert space, the Hamiltonian matrix is

$$H = \begin{pmatrix}
0 & -h & -h & 0 \\
-h & 4 & 0 & -h \\
-h & 0 & 4 & -h \\
0 & -h & -h & 4
\end{pmatrix}.$$  

The ground state wavefunction correct to order required for $h^3$ evaluation of Renyi entropies is

$$\psi_g = \left(1 - \frac{h^2}{8} - \frac{h^4}{576}\right) \left(\frac{h}{2} - \frac{h^3}{64}\right) \left(\frac{h^2}{8} + o(h^4)\right)$$  

Let $A_i$ label the basis states for subsystem $A$ and $B_k$ label basis states for subsystem $B$. Then reduced density matrix for subsystem $A$ has matrix elements

$$(\rho_A)_{A_i,A_j} = \sum_{B_k} \psi_{A_i,B_k} \psi_{A_j,B_k} \tag{S2}$$

In the TCM representation, there are just two states on the $A$ side, and the reduced density matrix becomes

$$\rho_A = \begin{pmatrix}
1 - \frac{h^2}{16} & \frac{h}{16} \\
\frac{h}{16} & \frac{h^2}{16} + \frac{h^4}{128}
\end{pmatrix}.$$  

From this it follows that the two eigenvalues of the reduced density matrix are $1 - \frac{h^2}{256}$ and $\frac{h^2}{128}$. It leads to Renyi entanglement entropy of

$$S_n^{(ii)} = \frac{1}{1-n} \left[-\frac{n h^4}{256} + \left(\frac{h^4}{256}\right)^n\right].$$  

Now, we turn to graph (i) in figure, which has 4 bonds all sharing a boundary site between $A$ and $B$. There are 4 plaquettes on which Visons can be created or destroyed. But, because they are created or destroyed in pairs, there number is conserved modulo 2. Thus, there are 8 relevant basis states. We can order the plaquettes in a clock- wise manner. Then the 8 states are: $|1\rangle = |0,0,0,0\rangle$, $|2\rangle = |1,1,0,0\rangle$, $|3\rangle = |0,1,1,0\rangle$, $|4\rangle = |0,0,1,1\rangle$, $|5\rangle = |1,0,0,1\rangle$, $|6\rangle = |1,1,1,1\rangle$, $|7\rangle = |1,0,1,0\rangle$ and $|8\rangle = |0,1,0,1\rangle$. The 8-dimensional Hamiltonian matrix is given by

$$H = \begin{pmatrix}
0 & -h & -h & -h & 0 & 0 & 0 & 0 \\
-h & 4 & 0 & 0 & -h & -h & -h & -h \\
-h & 0 & 4 & 0 & -h & -h & -h & -h \\
-h & 0 & 0 & 4 & -h & -h & -h & -h \\
0 & -h & -h & -h & 8 & 0 & 0 & 0 \\
0 & -h & -h & -h & 0 & 4 & 0 & 0 \\
0 & -h & -h & -h & 0 & 0 & 4 & 0
\end{pmatrix}.$$  

It leads to ground state wave function needed for 4th order calculation of Renyi entropies of:

$$\psi_g = \left(1 - \frac{h^2}{16} - \frac{9h^4}{64}\right) \left(\frac{h}{4} + \frac{h^3}{32}\right) \left(\frac{h^2}{4} + \frac{h^4}{32}\right) \left(\frac{5h^2}{8} + o(h^4)\right)$$

Transforming to the TCM variables $\sigma_z$, there are 4 states on the $A$ side, and remembering that each TFIM state is a superposition of two TCM basis states after applying the projection operator $(1+A_s)$, the $4\times4$ reduced density matrix becomes:

$$2\rho_A = \begin{pmatrix}
1 - \frac{h^2}{4} - \frac{9h^4}{64} & \frac{h}{4} + \frac{3h^3}{64} & \frac{h}{4} + \frac{3h^3}{64} & \frac{5h^2}{8} \\
\frac{h}{4} + \frac{3h^3}{64} & \frac{h^2}{8} + \frac{3h^4}{64} & \frac{h^2}{4} + \frac{3h^4}{64} & \frac{h}{4} + \frac{3h^3}{64} \\
\frac{h}{4} + \frac{3h^3}{64} & \frac{h^2}{8} + \frac{3h^4}{64} & \frac{h^2}{4} + \frac{3h^4}{64} & \frac{h}{4} + \frac{3h^3}{64} \\
\frac{5h^2}{8} & \frac{h}{4} + \frac{3h^3}{64} & \frac{h}{4} + \frac{3h^3}{64} & 1 - \frac{h^2}{4} - \frac{9h^4}{64}
\end{pmatrix}.$$  

From this it follows that the eigenvalues of $2\rho_A$ are $1 - \frac{3h^2}{4} - \frac{9h^4}{64}, 1 + \frac{3h^2}{4} + \frac{7h^4}{64}, \frac{h^2}{4}$ and $\frac{h^4}{64}$. These lead to Renyi entanglement entropies:

$$S_n^{(ii)} = \ln 2 - \frac{9h^4}{32} + \frac{1}{1-n} \left[(h^4/64)^n - n(h^4/64)\right].$$  

Note that this graph also gives the full line entropy of the unperturbed TCM, which is $\ln 2$ for every site that is shared between subsystems $A$ and $B$. For the unperturbed model, it is easily shown that any larger graph will give zero upon subgraph subtraction as no additional degeneracy arises on the line.

III. Kagome Heisenberg Model

The spin-1/2 Heisenberg model on the Kagome lattice, with both first- and second-neighbor interactions, is given by

$$H = J_1 \sum_{(ij)} S_i \cdot S_j + J_2 \sum_{(ij)} S_i \cdot S_j. \tag{S3}$$
FIG. S5: The entanglement entropy $S_n(L_y)$ for the Kagome $J_1$-$J_2$ model in Eq. (S3), with $L_y = 4 \sim 12$ at $L_x = \infty$. By fitting $S_n(L_y) = \alpha_n L_y - \gamma_n$, we get $\gamma_1 = 0.698(8)$ at $J_2 = 0.10$, and $\gamma_1 = 0.694(6)$ at $J_2 = 0.15$, while $\gamma_2 \approx 0.42(1)$ at both $J_2 = 0.10$ and 0.15. Here $n$ is the entropy index. Inset: Kagome lattice with $L_x = 12$ and $L_y = 8$. Here $S_i$ is the spin operator on site $i$, and $(ij) \langle \langle ij \rangle \rangle$ denotes the nearest neighbors (next nearest neighbors). In the numerical simulation, we set $J_1 = 1$ as the unit of energy. We take the kagomé lattice with periodic boundary conditions along a bond direction to define a cylinder, drawn vertically in the inset of Fig. S5 and the unit of length equal to the nearest-neighbor distance. The results for the entanglement entropy for $J_2 = 0.10$ and 0.15 are shown in Fig. S5, for which both spin-spin and dimer-dimer correlation lengths are approximately one lattice spacing. We see that a linear fit using data for $L_y = 4 \sim 12$ using Eq. (1) gives $\gamma_1 = 0.698(8)$ at $J_2 = 0.10$ and $\gamma = 0.694(6)$ at $J_2 = 0.15$, both within one percent of $\ln 2 = 0.693$. In contrast, the extrapolated TEE $\gamma_n$ based on the Renyi entropy (i.e., $n \geq 2$) clearly deviates from the expected value, although the cylinder’s circumference is much larger than the correlation length, i.e., $L_y \approx 10 \xi$. For example, as shown in Fig. S5, a linear fit using Eq. (1) gives us $\gamma_2 \approx 0.42(1)$ at both $J_2 = 0.10$ and $J_2 = 0.15$, which differs from the expected value by an $\approx 40\%$ error.