Accuracy of Topological Entanglement Entropy on Finite Cylinders

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Topological phases are unique states of matter which support nonlocal 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 a Z_2 topological ordered state using density-matrix renormalization group and perturbative series expansions. We find that extrapolations of the TEE based on the Renyi entropies with a Renyi index of $n \geq 2$ 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.

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Topological phases are exotic states of matter that are characterized by ground state degeneracy dependent upon global topology of the system on which the phase resides, and which host exotic excitations with fractional quantum statistics. In recent years, surprising connections have emerged between topological phases and quantum information, stimulated by the prospect of using them to construct an inherently fault-tolerant quantum computer [1,2]. Two-dimensional phases with topological order are well known in connection with the fractional quantum Hall effect [3], but are also expected to exist in frustrated quantum magnets [4,5].

While topological phases are not characterized by any *local* order parameter, theory shows that they can be identified by nonlocal quantum entanglement, specifically the topological entanglement entropy (TEE) of the ground states [6,7]. The entanglement entropy of a subregion A of the system with a smooth boundary of length L is defined from the reduced density matrix ρ_A, according to

$$S_1(A) = -\mathrm{Tr}[\rho_A \ln(\rho_A)],$$

and takes the form

$$S_1(A) = \alpha_1 L - \gamma,$$

where γ is the TEE. Severe finite-size corrections of the formulations in Refs. [6,7] due to lattice-scale effects greatly hinder their practical application [8]. Instead, two of us have recently proposed a practical and extremely simple scheme, the "cylinder construction," to accurately calculate TEE [9]. The cylinder construction simply consists of using the density-matrix renormalization group (DMRG) [10] to calculate the usual von Neumann entanglement entropy for the division of a cylinder into two equal halves by a flat cut, and extracting the TEE from its asymptotic large-circumference limit. Thereby, we can practically identify topological phases in arbitrary realistic models, including physical spin models [9,11].

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

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

while the von Neumann entropy S_1 is defined as the limit $n \to 1$. For simplicity, we will call S_n the Renyi entanglement entropy when $n \geq 2$, while the von Neumann entanglement entropy when $n = 1$. Theoretically, the universal TEE is expected to be obtained also for the Renyi entropy, with γ independent of the Renyi index [12,13]. 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 [14]. In particular, the extrapolated TEE in Ref. [14] from the second-order Renyi entropy S_2 deviates from the expected value with an error an order of magnitude larger than that from von Neumann entanglement entropy S_1 [9]. This suggests that extrapolations of Renyi entropies have significantly larger finite-size effects than von Neumann entropy.

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,

$$S_n(L) = \alpha_n L - \gamma_n, \tag{1}$$

as a function of the Renyi index n. First, we study the Toric-Code model whose TEE is known, using DMRG and perturbative series expansions [15]. 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 α_n varies more rapidly with parameters with increasing n. This makes the extraction of the subdominant γ_n term less reliable.

Toric-Code model.—We begin with the well-known Toric-Code model (TCM) [1] (see Supplemental Material [16] for notational details). Without applied fields, i.e., $h_x = h_z = 0$, the pure TCM is exactly soluble [1] with a Z_2 topological ordered ground state. After turning on the magnetic fields, the model is no longer exactly soluble. Previous studies [17–19] show that the Z_2 topological phase remains stable and robust until the magnetic fields are large enough that the system undergoes a phase transition from the topological phase to a trivial one. Numerically, Jiang, Wang, and Balents have systematically calculated the von Neumann entanglement entropy S_1 using cylinder construction [9], and extrapolated an accurate TEE $\gamma_1 = \ln(2)$ in the Z_2 topological phase, even very close to the phase transition point. In this Letter, we further calculate the Renyi entropy to study the finite-size effects on the TEE γ_n as a function of Renyi index n. To make sure that S_n only scales with the cylinder circumference $L_y = L$, we will work with long cylinder, i.e., cylinder length $L_x >> \xi$, where ξ is the spin-spin correlation length. For the present study, we consider the cylinder with length up to $L_x = 48$, which is $> \sim 40\xi$, e.g., for the pure electric case (i.e., $h_z = 0$) (see the Supplemental Material [16] for details). Therefore, we can directly extrapolate the TEE γ_n using Eq. (1).

To see the finite-size corrections, we first consider an applied magnetic field only along the x direction, i.e., $h_z = 0$. The extrapolated TEE γ_n are shown in Fig. 1(a) as a function of magnetic field h_x for fields within the topological phase. As shown in the Supplemental Material [16], for the fields in Fig. 1, the spin correlation length remains of order one lattice spacing or smaller. We see that the linear fit using data for $L_y = 6 \sim 12$ and Eq. (1) gives quite accurate results for γ_1 for $h_x < h_x^c \approx 0.328$ [17]. Even for $h_x = 0.3$, very close to the quantum phase transition, we obtain $\gamma_1 = 0.6945(20)$, which is accurate to the expected value (i.e., the dashed line) to a fraction of percent $\sim 0.2\%$. By contrast, the estimated TEE γ_n obtained from the Renyi entropy for $n \geq 2$ shows dramatically larger deviations from the universal value. These deviations grow when approaching the phase transition point, where the errors become an order of magnitude larger than those for γ_1. For example, $\gamma_2 = 0.714(5)$ at $h_x = 0.3$, with an error around $\sim 3\%$. The deviations also increase with Renyi index n, e.g., $\sim 7\%$ for $n = 4$, as shown in Fig. 1(a) and inset of Fig. 4. Similar results hold for the symmetric case $h_x = h_z$, with even larger finite-size corrections, as shown in Fig. 1(b) and the inset of Fig. 4. Systematically, the finite-size corrections to the TEE γ_n defined by Eq. (1) are much larger for the Renyi entropy than for the von Neumann entropy.

Our expectation is that in the thermodynamic limit $L_y \to \infty$, all γ_n should converge properly to the universal value. We look for signs of this tendency, by using a moving two data-point fit. We can define $\gamma_n(L_y)$ using two data points with different cylinder circumferences L_y and $L_y + 2$. Examples of such $\gamma_n(L_y)$ are shown in Fig. 2 for $h_x = 0.2$ and $h_z = 0$ in (a), and for $h_z = h_x = 0.2$ in (b), as a function of L_y. For both cases, $\gamma_1(L_y)$ and $\gamma_n(L_y)$ with $n \geq 2$ converge to the expected value with the

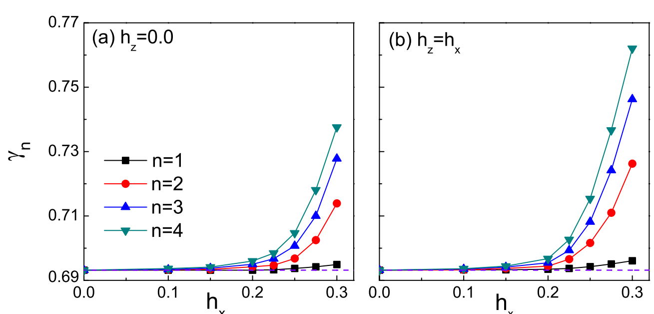

FIG. 1 (color online). The extrapolated TEE γ_n using von Neumann entropy (i.e., $n = 1$) and Renyi entropy (i.e., $n \geq 2$) for the Toric-Code model with $L_x = 48$, as a function of the applied magnetic field h_x, for (a) $h_z = 0$ and (b) symmetric case $h_z = h_x$. The dashed lines represent the expected universal value, ln2, for the TEE in the thermodynamic limit.

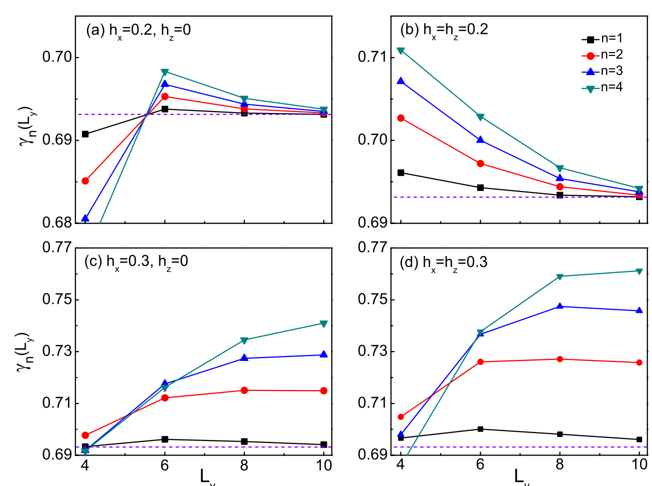

FIG. 2 (color online). Moving two point data fits for the extrapolated TEE γ_n for the Toric-Code model with $L_x = 48$ for (a) $h_x = 0.2$ with $h_z = 0$, (b) $h_x = h_z = 0.2$, (c) $h_x = 0.3$ with $h_z = 0$, and (d) $h_x = h_z = 0.3$, as a function of the cylinder circumference L_y and entropy index 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 $\gamma = \ln 2$.

increase of L_y, which is consistent with our expectation. Instead, for the other two cases, i.e., $h_x = 0.3$ and $h_z = 0$ in (c), and $h_z = h_x = 0.3$ in (d), $\gamma_1(L_y)$ quickly converges to the expected value, which is in sharp contrast to $\gamma_n(L_y)$ using Renyi entropies with $n \geq 2$. For the latter cases, the TEE is systematically overestimated. The curves in Fig. 2 do at least show downward curvature, also consistent with eventual convergence to the universal value for larger L_y, but it is clear that much larger systems would be required to test this in detail, due to a larger correlation length ξ (see Fig. S2 in the Supplemental Material [16]).

To understand the origin of the n dependence in the extrapolations, we turn to a perturbative series expansion calculation of the line term α_n. Since the TEE is obtained after subtraction of the much larger line term, an accurate extrapolation of γ_n also requires an accurate calculation of α_n. While there have been perturbative studies of the Kitaev model in a field [20] and some entanglement properties have also been studied [21,22], we are 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 [15].

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 nonzero[17] and on to a Z_2 lattice-gauge model if both h_x and h_z are nonzero [19]. In either case, one has a unique nondegenerate ground state. Here, we will consider only the former mapping and the case with only h_x nonzero. Up to 4th 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 [23]. 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 σ_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 [24,25]. The entanglement entropies can be expressed as

$$S_n = \sum_c W_n(c), \tag{2}$$

where the sum is over all possible clusters c and the weight of a cluster $W_n(c)$ is defined recursively by the relations

$$W_n(c) = S_n(c) - \sum_s W_n(s), \tag{3}$$

where $S_n(c)$ is the entanglement entropy for the cluster c and the sum over s is over all subclusters of c.

One can show that, for the line entropy, the only clusters that will give nonzero contributions in powers of h are those that are (i) linked and (ii) that contain at least one bond in subsystem A and one in subsystem B [24,25]. 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 Supplemental Material [16].

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

$$\alpha_n = \frac{1}{2}\left(\ln 2 - \frac{9n}{32}h^4 + \frac{3n}{n-1}\frac{h^4}{128}\right), \tag{4}$$

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

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

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 nonzero as a power of the perturbation parameter.

In. Fig. 3 we show the line entropies α_n obtained in DMRG compared with the series expansion results (See also Fig. S3 in the Supplemental Material [16]). The

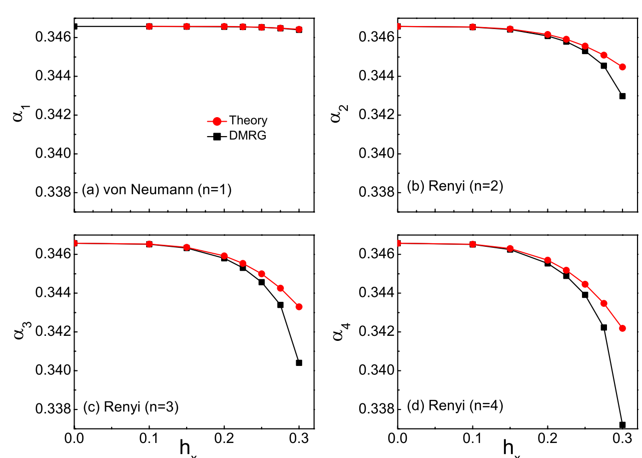

FIG. 3 (color online). Line entropy α_n obtained from DMRG (block square) and perturbative calculation (red circle) for both von Neumann entropy (i.e., $n = 1$) and Renyi entropy (i.e., $n \geq 2$) for the Toric-Code model, as a function of the magnetic field h_x, here $h_z = 0$ and $L_x = 48$.

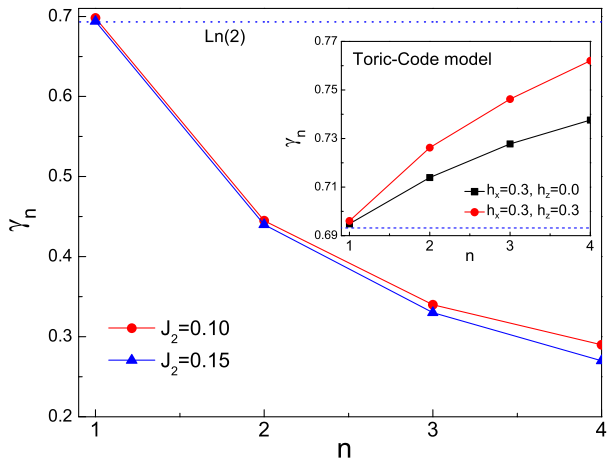

FIG. 4 (color online). The extrapolated TEE γ_n for the kagome J_1-J_2 Heisenberg model as a function of entropy index n at both $J_2 = 0.10$ and $J_2 = 0.15$. Inset: γ_n for TCM as a function of entropy index n, for the case $h_x = 0.3$, $h_z = 0$ (black square), and the symmetric case $h_x = h_z = 0.3$ (red circle). The dashed lines correspond to ln(2).

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 [26,27] and direct evidence [9,14] for a topological quantum spin liquid has been obtained by extensive DMRG studies, consistent with a Z_2 topological state [28–30]. Additional phenomenological predictions for the Z_2 state have appeared [31,32], and are also in agreement with DMRG results. Furthermore, accurate TEE $\gamma_1 = \ln(2)$ has been obtained using cylinder construction [9], for the model with both first- and second-neighbor interactions—see the Supplemental Material [16] for details of the definition. Specifically, the extrapolated TEE $\gamma_1 = 0.698(15)$ at $J_2 = 0.10$ and $\gamma_1 = 0.694(12)$ at $J_2 = 0.15$, both within 1% of $\ln(2) = 0.693$.

As in the TCM, we find that the Renyi entropies give much less accurate estimates of γ_n. The extrapolated TEE γ_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. S5, a linear fit using Eq. (1) gives $\gamma_2 \approx 0.44(2)$ at both $J_2 = 0.10$ and $J_2 = 0.15$: a huge error of ~40%. Moreover, with increasing Renyi index n, the deviation becomes even larger, reaching, for example ~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 Letter, 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 10 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 the 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 α_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 is obtained 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 Letter we have focused on systems with Z_2 topological order, similar conclusions may be expected more generally.

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