Topological transitions from multipartite entanglement with tensor networks: sharper and faster

Román Orús, Tzu-Chieh Wei, Oliver Buerschaper, and Artur García-Saez

1Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany
2C. N. Yang Institute for Theoretical Physics, State University of New York at Stony Brook, NY 11794-3840, USA
3Perimeter Institute for Theoretical Physics, 31 Caroline Street North, Waterloo, Ontario, Canada, N2L 2Y5

Topological order in a 2d quantum matter can be determined by the topological contribution to the entanglement Rényi entropies. However, when close to a quantum phase transition, its calculation becomes cumbersome. Here we show how topological phase transitions in 2d systems can be much better assessed by multipartite entanglement, as measured by the topological geometric entanglement of blocks. Specifically, we present an efficient tensor network algorithm based on Projected Entangled Pair States to compute this quantity for a torus partitioned into cylinders, and then use this method to find sharp evidence of topological phase transitions in 2d systems with a string-tension perturbation. When compared to tensor network methods for Rényi entropies, our approach produces almost perfect accuracies close to criticality and, on top, is orders of magnitude faster. The method can be adapted to deal with any topological state of the system, including minimally entangled ground states. It also allows to extract the critical exponent of the correlation length, and shows that there is no continuous entanglement-loss along renormalization group flows in topological phases.

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Topological order [1] is a striking property of quantum matter beyond the Landau paradigm and is characterized by an underlying pattern of long-range entanglement. The existence of such a pattern can be detected, quantitatively, by the so-called topological entanglement entropy $S_T$ [2]. Other entanglement properties are sensitive to topological order as well [3]. Moreover, under the effect of a local perturbation it is also well-known that topological order is generally robust [4, 5] and can sustain a finite perturbation. Intuitively, large closed strings and string-nets become energetically expensive in a topological phase as a string-tension is increased, thus ultimately favoring a transition towards a topologically-trivial phase. A drawback of using entanglement to detect such topological transitions, however, is that it is very difficult to produce sharp numerical evidence. The reason for this is that commonly used methods, such as the calculation of the topological contribution in Rényi entropies [6], suffer from a significant drop in accuracy when close to a quantum critical point [7], see Fig.1. Here we show how multipartite entanglement, in combination with tensor networks, improves accuracies to an almost perfect level and, on top, is computed orders of magnitude faster than any Rényi entropy.

More specifically, here we use a novel and efficient tensor network method to evaluate the topological contribution to the geometric entanglement (GE) of blocks, which we call $E_T$, for a torus partitioned into cylinders. When close to a quantum phase transition, we find that this approach completely outperforms in accuracy and efficiency calculations of Rényi entropies on infinite cylinders with tensor networks [29]. Without describing the technical details, the main result is summarized in Fig.1. We apply a string tension $g$ (which corresponds to a magnetic field in the Hamiltonian [8, 9]) to certain toric code ground states, and compute the topological contribution of the GE of these “strained” toric code states. Unlike the topological Rényi entropies, the computed $E_T$ stays close to $-1$ throughout the entire topological phase and, as the string tension increases, it sharply drops down to zero at $g^* \approx 0.56$ and remains there in the trivial phase. From a mapping to a classical 2D Ising model [8] we obtain...
analytically a transition at $g^* = \sqrt{1 + \sqrt{2}} - 1 \approx 0.5537$, in agreement with the above. $E_\gamma$ is thus an excellent tool to pinpoint topological phase transitions.

Our method uses Projected Entangled Pair States (PEPS) [12]. If the PEPS is topological [13], then a robust $E_\gamma$ is extracted via finite-size scaling for large toruses. For non-trivial partitions we find $E_\gamma$ to depend on the particular superposition of ground states on the torus, in agreement with the behavior of Rényi entropies [14]. Our calculations focus mainly on PEPS with a translation invariant representation. This has two main advantages: first, it simplifies the calculations, and second, it corresponds to the type of unique ground state of a topological system that can be found on an infinite plane using, e.g., the iPEPS method [15]. Even if such states have a weaker topological contribution on a torus than minimally entangled states (MES), they are much simpler to deal with, and already produce non-trivial topological contributions. In any case, we shall see that our method can be easily extended to PEPS representations that are not invariant under translations, thus including MES if necessary. Importantly, with this method we also have access to other properties. For instance, in the supplementary material we show how to extract the critical exponent $\nu$, and how to see that there is no continuous entanglement-loss along renormalization group flows in topological phases [16].

GE and topological GE — The geometric entanglement of blocks [17, 18] has recently proven useful to assess topological order [19]. This multipartite measure has been extensively used in quantum phase transitions [20], and can be measured experimentally, e.g., in NMR [21] and potentially in optical lattice experiments [22]. In contrast to all other entanglement approaches for topological matter, the GE takes into account the multipartite structure of entanglement in quantum many-body states. It amounts to computing the closest product state $|\Phi\rangle$ to a given quantum state $|\Psi\rangle$ in the Hilbert space, where the product state has a separable structure of $n_b$ blocks, i.e., $|\Phi\rangle = \prod_{i=1}^{n_b} |\phi^{(i)}\rangle$. It thus quantifies the merit of a possible mean-field description of the quantum state. Conveniently, the GE is defined as $E_G = -\log |\langle \Phi | \Psi \rangle|^2$.

One of the latest findings has been that, for renormalization group (RG) fixed points such as the toric code and other topological exactly-solvable models, the GE of blocks obeys $E_G = E_0 - E_\gamma$, with $E_\gamma$ a topological contribution (the topological GE) and $E_0$ some non-universal term [19]. It was observed that $E_\gamma = S_0$ for the considered models. As for $E_0$ it was found that $E_0 \propto n_b L$, with $n_b$ the number of blocks with a contractible boundary of size $L$. Moreover, under perturbations it was argued that $E_G = E_0 - E_\gamma + O(L^{-\nu'})$ for $L \gg 1$, where again $E_0 \propto n_b L$, $\nu'$ is some exponent, and $E_\gamma$ is the (robust) topological term. However, the validity of this equation was based so far on small-size calculations and qualitative RG arguments. Here we confirm and extend the validity of this relation by computing $E_\gamma$ for large-size perturbed topological 2d models using blocks with non-contractible boundaries.

Computing $E_G$ and $E_\gamma$ from a PEPS — Our approach to computing the GE of non-contractible blocks $E_G$ for large block sizes and its topological contribution $E_\gamma$ uses 2d PEPS and 1d Matrix Product States (MPS). Both PEPS and MPS have been widely discussed in the literature (see, e.g., Ref.[23]). It is worth mentioning that PEPS can describe 2d topological phases naturally, both chiral [24] and non-chiral (or doubled) [13]. For simplicity, here we focus on non-chiral topological order, but a generalization of our method to chiral models is also possible.

As a starting point we assume that a PEPS $|\Psi\rangle$ with (potentially) topological order is given on a torus of $n \times L$ sites, see Fig.2(a). We call such a state $|\Psi(n, L)\rangle$. This PEPS could be the result of an analytical derivation, or have been computed numerically from a Hamiltonian using, e.g., the iPEPS algorithm [15] and wrapping later its tensors around a finite torus.

The goal now is to extract $E_G$ and $E_\gamma$ from such a PEPS. With this in mind, we partition the torus into $n_b$ cylinders of equal width $L = n/n_b$. Thus each cylinder contains $l \times L$ sites, see, e.g., Fig.2(b). This choice of partition will have a double benefit. First, it will simplify the tensor contractions in the method. Second, it will be sensitive to different ground states on the torus, and hence to MES.

We focus on the case $l = 1$, so that $n_b = n$. In this
In what follows we describe an optimization procedure, well-suited for gapped topological phases, to solve this problem. The method assumes a translation invariant PEPS, but it can also be generalized to states without translation symmetry (such as MESs).

1. Assume translation invariance so that cylinders are repeated periodically. While not necessary for a finite system, this assumption simplifies the calculations and also produces good results for translation invariant PEPS. Here a 2-cylinder unit-cell is already sufficient, but bigger unit cells can also be considered.

2. Fix all tensors in the MPSs to some initial (e.g., random) values except for one cylinder, and optimize variationally the MPS tensors for that cylinder. The result of this optimization is given by the diagram in Fig.2(c,d). Notice, though, that for a 2d lattice the environment tensor $E$ cannot be computed both exactly and efficiently, and therefore needs to be approximated.

3. Compute an effective environment $\tilde{E}$ approximating the exact environment $E$, using some method to approximate contractions of 2d tensor networks. In our case we assume further translation invariance within each cylinder, and use the iTEBD method for non-unitary evolutions [25, 26], forgetting about the periodic boundary conditions imposed by the torus geometry, and adapted to deal with Matrix Product Operators (MPO). The specifics are explained in the supplementary material. As a result of this approach, an infinite MPO of bond dimension $\chi$ is produced which is then cut at length $L$ and wrapped around a circle with pbc. Such an approximation is particularly accurate for large $L$ and gapped phases, which is precisely the regime of interest to extract $E_\gamma$. This finite MPO with pbc describes the effective environment $\tilde{E}$, see Fig.2(e).

4. Approximate the optimal MPS for the cylinder as in Fig.2(f).

5. Substitute this MPS in all the equivalent cylinders by translation invariance.

6. Repeat the procedure for the next cylinder in the unit cell.

7. Iterate until convergence.

The optimal overlap is thus evaluated as

$$\Lambda_{\text{max}}(n, L) \approx \frac{|\langle \Phi | \Psi(n, L) \rangle|}{\sqrt{|\langle \Phi | \Phi \rangle||\langle \Psi(n, L) | \Psi(n, L) \rangle|}}, \quad (1)$$

with $|\Phi \rangle = \otimes_{i=1}^{n} |\phi^{[i]}\rangle$, and $|\phi^{[i]}\rangle$ the optimal MPS for each cylinder. In this expression, the numerator can be approximated using, e.g., the procedure described in the first section of the supplementary material with a computational cost of $O(n_\delta \chi^3 D^5 + L \chi^3)$. The norm of $|\Phi\rangle$ is simply the product of the norms of the $n_\delta$ MPS of size $L$ with pbc, which can be evaluated exactly and efficiently in $O(L \chi^5)$ steps (see, e.g., [23]). The norm of the $n \times L$ PEPS $|\Psi(n, L)\rangle$ can be approximated as in the first section of the supplementary material with a computational cost of $O(n \chi n^2 D^9 + \chi^3 D^6 + L \chi^6)$, with $n'$ the bond dimension of the needed MPO. Finally, the GE is given by $E_G(n, L) \equiv -\log_2 \Lambda_{\text{max}}^2(n, L)$.

For an $n \times L$ PEPS on a torus it is thus possible to approximate $E_G(n, L)$ as above. To get the topological contribution, the next step is to perform finite-size scaling with respect to $n$ and $L$. In particular, we have $E_G(n \gg 1, L \gg 1) \sim a n L - E_\gamma(n, L)$, where $E_\gamma(n, L)$ includes both the topological component $E_\gamma$ as well as finite-size corrections. We can then fix $n$ and compute $E_G(n, L)$ for increasing $L$. Doing a linear fit for large $L$ allows us to extract an approximation to the topological GE by extrapolating the fit down to $L = 0$. The larger $n$ is, the more accurate the approximation is. Thus, the value of the topological correction is finally estimated as $E_\gamma = \lim_{n, L \to \infty} E_\gamma(n, L)$.

Some remarks are in order. First, accuracy can always be improved by increasing the different bond dimensions, or by applying tensor network methods that explicitly take into account pbc rather than iTEBD, or by using larger unit cells (and even breaking completely translation invariance along any direction) in the product state $|\Phi\rangle$. Second, cylinders of larger width $l > 1$ can be considered by using a PEPS for an $l$-leg ladder with pbc to approximate the state $|\phi^{[i]}\rangle$ within each cylinder, or perhaps even an MPS with pbc and physical dimension $d'$.
(d) corresponds to the unperturbed toric code on a square lattice at the same critical point, showing that the transitions in the same perturbation is applied to different ground states on the honeycomb lattice. Notice that (b) and (c), though being ground states on the same lattice, have different transition points. This is because the string tension $g$ was applied in different bases, hence corresponds to different physical perturbations. However, we have also checked that, when the same perturbation is applied to different ground states on the same lattice, the topological phase transition takes place at the same critical point, showing that the transitions in $E_\gamma$ do not depend on the specific choice of ground state. Figure (d) corresponds to the unperturbed toric code on a square lattice for two different ground states: an MES $|\Xi_0\rangle$, and a non-MES $|0,0\rangle$.

(with $d$ the physical dimension of a single site). An example of such a calculation is shown in the supplementary material. Third, MESs can also be studied introducing minor changes in the method. For this, notice that the PEPS representation of an MES is translation invariant except for, e.g., one cylinder where a Wilson loop operator acted. Thus, one chooses $|\Phi\rangle$ as a translation invariant product state of MPSSs, except for the Wilson loop cylinder, where a different MPS is chosen. The rest of the method just follows.

**Topological phase transitions from $E_\gamma$** — Using the above method we computed $E_{C_2}$ and $E_\gamma$ for the toric code model [4] with string tension on the square and honeycomb lattices. Details about the PEPS for these models are given in the supplementary material. The string tension $g$ drives the systems towards a phase transition between topological and polarized phases. Using the notation from Ref.[19], we considered perturbations to two non-equivalent ground states $|0,0\rangle$ and $|+,+\rangle$ for the honeycomb lattice, whereas for the square lattice we considered perturbations to the $|0,0\rangle$ state. In the topological phase, these states are the unique ground states of the system on an infinite plane, but on a torus they correspond to a superposition of MESs with topological entropy $S_\gamma = -1$ for a non-contractible bipartition [14].

Our calculations were done for toruses up to $n = 100$ and $L = 100$. Larger sizes could have easily been considered if necessary. In Fig.3 we show an example of the scalings with $L$ for different values of $n$ up to $n = 20$ for two different string tensions $g = 0.4, 0.6$ on the square lattice. The linear fit is computed from the last half of $L$ values, which produces robust results. In the plots, the extrapolation of the fit to $L = 0$ hits the vertical axis around $-1$ if $g$ is small, corresponding to the topological phase, and around $0$ for large $g$, corresponding to the polarized phase. From the fits we can extract $E_\gamma$, as a function of $n = n_b$ and $g$, as shown in Fig.4(a-c) for the three states considered. Remarkably, these plots show very sharp indications of topological phase transitions for all these models for large $n_b$. With this approach we also extracted $E_\gamma$ for one of the MES of the square lattice toric code on a torus without perturbation. Specifically, we considered the state $|\Xi_0\rangle \equiv 2^{-1/2}(|0,0\rangle + |1,0\rangle)$ (in the notation of Ref.[19]) which has $S_\gamma = -2$ for a non-trivial torus bipartition [14]. Remarkably, we also find $E_\gamma = -2$ for this state, see Fig.4(d).

**Conclusions** — We computed sharp evidence of topological quantum phase transitions for 2d systems, by calculating $E_\gamma$ using a new and efficient tensor network method for non-trivial partitions on a torus. Our method completely outperforms similar tensor network calculations of Rényi entropies for infinite cylinders, by being orders of magnitude more accurate and efficient close to criticality [7]. This approach can also be applied to different ground states, including MES, and allows to extract other non-trivial information about the system (e.g., correlation length critical exponent, and lack of continuous entanglement loss along RG flows in topological phases). Our work motivates further research along several directions. For instance, it would be possible to use these tools to study chiral topological order [27], topological critical exponents, and MES. Beyond tensor network methods, it would be interesting to study how to compute $E_\gamma$ using Quantum Monte Carlo, and compare the accuracy and efficiency to that of 2-Rényi entropy calculations. A general investigation of arbitrary ground states on a torus, including $E_\gamma$ for MES, will appear in a separate publication [28].

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SUPPLEMENTARY MATERIAL

In this supplementary material we provide details on the following:

1. Tensors for the toric code model with string tension on different lattices.
2. Calculation of the effective environment using iTEBD and MPOs.
3. Extracting $E_\gamma$ using cylinders of width $l = 2$ on the square lattice.
4. Alternative optimization strategies and finite-size effects in $E_G$.
5. Fidelity diagram and no entanglement loss along RG flows in topological phases.
6. Extracting the critical exponent $\nu$ from the finite-size scaling of $E_\gamma$.
7. Efficient methods to compute the $n$-th-Rényi entropy and its topological contribution, for finite and infinite $n$, for a 2d PEPS on an infinite cylinder.

1. Tensors for the toric code with a string tension

As examples of perturbed topological models, in this paper we have considered Kitaev’s toric code model [3] with a string tension on square and honeycomb lattices. It is well known that the ground states for these systems on an infinite plane can always be specified by a PEPS. Here we adopt the convention that tensor bond indices are subscripts, starting from the leftmost index in the lattice and following a clockwise rotation order, and physical indices are superscripts. According to this convention, and following the notation of Ref.[4] for the toric code ground states, the three PEPS that we consider here are:

(i) Perturbed $|0, 0\rangle$ ground state on the square lattice. This is described by 2 PEPS tensors $A$ and $B$ with bond dimension $D = 2$. The non-zero coefficients $A_{i\alpha\beta\gamma\delta}$ (where $i$ and $\alpha \ldots \gamma$ are the physical and bond indices respectively) are given by

\[
A_{1,1,1,1}^1 = 1 + g \quad A_{2,2,1,1}^2 = 1 \\
A_{2,2,2,2}^1 = 1 + g \quad A_{1,1,2,2}^2 = 1
\]  

(2)

with $g$ a string tension, and $B$ being a rotation of $\pi/2$ of $A$ on the lattice.

(ii) Perturbed $|0, 0\rangle$ ground state on the honeycomb lattice. This is described by two tensors $T$ and $\Delta$ with non-zero coefficients

\[
T_{1,1}^1 = 1 + g \quad T_{1,2}^2 = 1 \\
T_{2,2}^1 = 1 + g \quad T_{2,1}^2 = 1
\]  

(3)

and

\[
\Delta_{1,1,1} = \Delta_{2,2,2} = 1.
\]  

(4)

see Fig.5. A more convenient description for the numerical calculations is given in terms of tensors $A$ and $B$ computed from $T$ and $\Delta$ as shown in Fig.5. In this construction the PEPS bond dimension is $D = 2$, whereas the physical dimensions are 2 for $A$ and 4 for $B$.

(iii) Perturbed $|+, +\rangle$ ground state on the honeycomb lattice. This is described by tensors $T, \Delta$ and $\tilde{\Delta}$ with non-zero coefficients

\[
T_{1,1}^+ = 1 + g \quad T_{2,2}^- = 1 \\
T_{4,4}^+ = 1 + g \quad T_{3,3}^- = 1
\]  

(5)

\[
\Delta_{1,1,1} = \Delta_{3,3,1} = \Delta_{2,1,3} = \Delta_{1,2,2} = 1 \\
\Delta_{4,3,3} = \Delta_{3,4,1} = \Delta_{2,2,4} = \Delta_{4,4,4} = 1
\]  

(6)
FIG. 5: (color online) tensors for the PEPS $|0,0\rangle$ perturbed ground state on the honeycomb lattice. The lattice is represented as a brickwall.

FIG. 6: (color online) tensors for the PEPS $|+,+\rangle$ perturbed ground state on the honeycomb lattice. The lattice is represented as a brickwall.

\[ \tilde{\Delta}_{1,1} = \tilde{\Delta}_{3,3} = 1, \quad \tilde{\Delta}_{1,2} = \tilde{\Delta}_{2,1} = 1, \]
\[ \tilde{\Delta}_{3,4} = \tilde{\Delta}_{4,3} = 1, \quad \tilde{\Delta}_{2,4} = \tilde{\Delta}_{4,2} = 1, \]  

(7)

see Fig. 6. One can rewrite again the tensor network in terms of two tensors $A$ and $B$ as shown in Fig. 6. This time, the PEPS bond dimension is $D = 4$, and the physical dimensions are again 2 for $A$ and 4 for $B$.

Remarks

The above perturbations on the $|0,0\rangle$ and $|+,+\rangle$ states on the honeycomb lattice correspond, in fact, to different physical perturbations: one adds weight to strings of 1’s or +’s respectively. It is, however, easy to apply the same perturbation to both ground states. For instance, in the $\{|1\rangle, |2\rangle\}$ basis for every spin, the perturbed $|0,0\rangle$ state can be written as $Q \otimes N |0,0\rangle$, with $N$ the number of spins and $Q = (1 + g)|1\rangle\langle 1| + |2\rangle\langle 2|$. The perturbed $|+,+\rangle$ state after applying the same perturbation $Q$ to every spin then reads $Q \otimes N |+,+\rangle$, and the PEPS for such a state is easy to compute in the $\{|+, -\rangle\}$ local basis (with $|\pm\rangle = (|1\rangle \pm |2\rangle)/\sqrt{2}$) and noticing that the perturbation operator can be written as $Q = (1 + g/2)(|+\rangle\langle +| + |-\rangle\langle -|) + (g/2)(|+\rangle\langle -| + |-\rangle\langle +|)$.

2. Computation of the effective environment $\tilde{E}$ as an MPO using iTEBD

At several points in our numerical methods we use iTEBD to produce an MPO approximation of the multiplication of several transfer operators, e.g., when computing the exact environment $E$ for $E_G$ in step 3. To do so, we assume that we have translation invariance every, e.g., 2 lattice sites at least. This MPO is produced is as follows:

1. Contract the tensors for two columns as in Fig. 7(a). This is the product of two infinite MPOs. If both MPOs have bond dimension $D$, then the resulting MPO will have bond dimension $D^2$.

2. Find the canonical form of the resulting MPO, see Fig. 7(b,c). This can be done using the algorithms from Ref.[1, 2], adapted to an MPS with two physical legs per site of dimension $D$ each.

3. Truncate the bond dimension of the MPO to its largest $\chi'$ Schmidt coefficients of a bipartition across each link, see Fig. 7(d).

4. Absorb the Schmidt coefficients into the tensors at each site, see Fig. 7(e).
5. *Iterate* until approximating the contraction of \( n_b - 1 \) infinite columns. At each iteration step we will have as input two infinite MPOs, one of bond dimension \( \chi' \) and another one of bond dimension \( D \). The output will always be a new infinite MPO of bond dimension \( \chi' \).

![Diagram](image)

**FIG. 7:** (color online) iTEBD method for non-unitary MPOs, adapted from Ref.[2]. (a) Contraction of 2 MPOs of bond dimensions \( \chi' \) and \( D \). (b) Resulting MPO of bond dimension \( D\chi' \). (c) Canonical form of the MPO in (b), in terms of MPO tensors (circles) and matrices of Schmidt coefficients (diamonds). (d) Truncated MPO of bond dimension \( \chi' \) in canonical form. (e) Final MPO, were we have absorbed the Schmidt coefficients into the tensors at each site.

3. Extracting \( E_\gamma \) using cylinders of width \( l = 2 \)

As a proof of principle, we have done a calculation for cylinders with a width of more than one site, namely \( l = 2 \). For toruses up to 100 × 100 sites, this implies that \( n_b \) reaches up to 50 cylinders. In Fig.8 we see an example of such a calculation for the perturbed toric code ground state on the square lattice, and compare it to that of Fig.4(a). As expected, we see convergence with \( n_b \) twice as fast as compared to the case \( l = 1 \), showing the same estimation for the quantum critical point \( g^* \approx 0.56 \).

![Graph](image)

**FIG. 8:** (color online) \(|E_\gamma|\) extrapolated from the scaling with \( L \), as a function of the string tension \( g \) and the number of cylinders \( n_b \), for toruses up to 100 × 100 sites, for the perturbed toric code on a square lattice and cylinders of width (a) \( l = 1 \), and (b) \( l = 2 \). Notice that both plots look almost identical, but the vertical axis in (b) spans half the values of the vertical axis in (a).

4. Alternative optimization strategies and finite-size effects

The numerical optimization of tensors presented in the main text deals directly with systems of infinite size and then wraps them around a finite-size torus. Here we explore the alternative option of optimizing the tensors in the product state approximation to \(|\Psi(n, L)|\) directly on a torus, i.e., implementing the effect of periodic boundary conditions. We expect this optimization to be less efficient, therefore we can only access system sizes smaller than the ones mentioned in the main text. However, we also expect that finite-size corrections are more accurate, especially
FIG. 9: (color online) $E_\gamma$ estimated from the finite-size optimization, for the square lattice toric code state $|0, 0\rangle$, as a function of the string tension $g$ and $n = 10 \ldots, 18$. (a) $L = 20$, and (b) $L = 30$. Notice that there is a strong dependence on $L$, especially around the transition region. As expected, larger systems show a more robust topological phase, in turn tending towards the results in the main text for $L \gg 1$, which are represented by a black solid line.

FIG. 10: (color online) $R^2$ for the linear fit. We observe that only at small system sizes the fit slightly deviates from almost-perfect linearity. The largest deviation is around the transition point, and vanishes for increasing system sizes.

around the phase transition point. Thus, this is a valid and precise option to study finite-size corrections in $E_G$ for small- and medium-size systems.

To check the validity of this “finite-size” optimization using MPSs for each cylinder, we have checked that we obtain essentially the same results as the exact optimization, where no MPS approximation is used for the cylinders. This calculation, thus, validates our MPS approximation for the states within each cylinder. For toruses up to $L \approx 10$ and $n \gg 1$, we recover essentially the same results whenever the MPS bond dimension fulfills $\chi \approx 10 - 12$ (results not shown). Once this is clear, we have proceeded with the “finite-size” optimization over MPSs for larger toruses. As one can see in Fig.9, there is a strong dependence of $E_\gamma$ on the system size in the transition region, as expected. This can be used as an extra justification for the method used in the main text, which hits very efficiently the infinite-size limiting behavior even around the transition region. In a nutshell, by using systems of large size we rule out the possibility of any finite-size effect coming either from the optimization of the tensors or from the finite-size scaling on the torus.

In this work we have computed $E_\gamma$ assuming a linear scaling with $L$ for $E_G$ and large $L$. Here we justify this approach by showing that non-linear corrections vanish in the large-size limit. We test directly the validity of the linear fit by computing its coefficient of determination $R^2$. This is shown in Fig.10, for systems up to $L = 20$ and $n_b = 30$. The plot shows $R^2$ as a function of $g$ and $n_b$, and one can see that a significant deviation from a perfect linear fit (for which $R^2 = 1$) happens only close to the transition point, and in fact vanishes as the system size increases.

Finally, in order to assess the validity of the linear fit we can also study deviations from it, e.g.,

$$E_G = E_0 - E_\gamma + O(L^{-1}) + O(L^{-2}),$$  \hspace{1cm} (8)
which introduces non-linear terms in the fit. In Fig.11 we plot the coefficients for the $O(L^{-1})$ and $O(L^{-2})$ contributions to Eq.8. We see that the presence of these two terms is only significant for small systems around the transition point, vanishing for large system sizes. Notice also that the results shown in the main text were obtained for large systems, so that these non-linear contributions should be negligible. Such finite-size effects are only accessible in small- and medium-size systems, as shown here.

5. No continuous entanglement-loss in topological phases and local fidelity

In Ref.[5] it was argued that 1d many-body systems with conformally-invariant quantum critical points display continuous entanglement-loss along RG flows between fixed points. This was understood as a refinement of Zamolodchikov’s famous c-theorem [6], recently generalized to 2d [7]. However, recent works have shown counter-examples to this behavior for different systems [8]. Here we provide similar results using the density of GE per block, which for large $L$ corresponds to the linear term in our fits. To determine the nature of the RG flows in our systems, we computed the local fidelity diagram in Fig.12(a) [9]. The pinch-point in the local fidelity $d(g_1, g_2)$ [10] is in accordance with a continuous phase transition at $g^* \approx 0.6$, in turn corresponding to a critical and non-topological RG fixed point. Two more non-critical fixed points are present at $g = 0$, which is topological, and $g = \infty$, which is trivial. Coarse-graining drives the quantum state towards either $g = 0$ or $g = \infty$ depending on the phase, and thus $g = g^*$ is an unstable fixed point. As for the density of GE per block, in Fig.12(b) we see that, in the topological phase, it increases as we move away from the phase transition point, so that the entanglement per site rises when flowing from $g = g^*$ towards $g = 0$. Albeit not a universal contribution, this already implies that there is no continuous reordering of quantum correlations at every infinitesimal RG step along the corresponding RG flow between these two fixed points, which rules out the possibility of continuous entanglement loss in the wave function.

6. Correlation length critical exponent $\nu$ from $E_\gamma$

Near criticality the only relevant length scale in the system is the correlation length, which scales as $\xi \sim |g - g^*|^{-\nu}$. For a finite-size system, the estimate $g_c$ of the critical point $g^*$ will depend on the system size $L_s$: $|g_c - g^*| \sim L_s^{-1/\nu}$. In our case, we have two different sizes $n_b$ and $L$. If we take $L$ very large, the remaining finite length-scale will be given by $n_b$, and thus in our case $|g_c - g^*| \sim n_b^{-1/\nu}$. We can test such an ansatz scaling to estimate the critical exponent $\nu$ from the behavior of $E_\gamma(n_b, L \to \infty)$, i.e., from the data in Fig.4(a-c).

For instance, consider the perturbed toric code on the square lattice (Fig.4(a)). For $n_b$ between 12 and 60 we find that the best fit is $g_c = 0.55 + 3.83/n_b^{1.34}$ with $R^2 = 0.99992$, thus $\nu \sim 1/1.34$ (Fig.13(a)). Between $n_b = 40$ and 60, the best fit gives $g_c = 0.55 + 5.58/n_b^{1.48}$ with $R^2 = 0.99999$, giving $\nu \sim 1/1.48$, close to 2/3 (Fig.13(b)). The critical exponent $\nu$ is thus estimated to fall roughly between 0.68 and 0.75. For comparison, other values found in topological transitions for the square-lattice toric code model are the Ising value $\nu \sim 0.63$ for a parallel magnetic field, and also
any value between $\nu \sim 0.63$ and $\nu \sim 1$ along a multicritical line for an arbitrary field [11]. In our case, we believe that errors come from the finite number of grid points for $g$ and the procedure of estimating $g_c$ (which we determine as the value of $g$ at $|E_\gamma| \sim 0.5$ by interpolating the available data). The accuracy can be improved by computing more data, but in any case, the analysis suggests that the transition is continuous, in accordance with our fidelity results in Fig.(12).

7. Tensor network methods to compute Rényi entropies on infinite cylinders

The Rényi entropy between a subsystem with reduced density matrix $\rho$ and the rest of the system is given by

$$S^{(n)} = \frac{1}{1-n} \log \left( \text{tr} \left( \rho^n \right) \right),$$

with $n$ the Rényi entropy index. The limit $n \to 1$ coincides with the usual von Neumann (or entanglement) entropy $S^{(1)} = -\text{tr} \log \rho$, whereas the limit $n \to \infty$ corresponds to the so-called infinity Rényi entropy, or single-copy entanglement, $S^{(\infty)} = -\log \nu_1$, with $\nu_1$ the largest eigenvalue of $\rho$. In Ref.[12] it was proven that all these entropies have the same topological contribution, so that any of them can be used to identify the topological nature of a given state.

Because of this, in combination with their apparent simplicity, Rényi entropies have become quite common tools to evaluate the presence of topological order in quantum many-body systems. For instance, the 2-Rényi entropy is a usual approach in Quantum Monte Carlo [13], whereas in tensor networks, and especially in 2d PEPS, both the the 2-Rényi entropy and the infinite Rényi entropy (or single-copy entanglement) are easily accessible quantities. This follows, e.g., from the approach explained in Ref.[14], which relies on wrapping the 2d PEPS around a cylinder of circumference $L$, and considering a non-contractible bipartition of the cylinder in two halves.
Let us be more precise with the tensor network calculation: we start with a 2d PEPS $|\psi(L)\rangle$ on a cylinder of circumference $L$. For simplicity, we assume that the cylinder is infinitely long, though finite systems can also be considered easily. We partition the cylinder into two half-infinite pieces $A$ and $B$, see Fig.14(a). As explained in Ref.[14], the reduced density matrix of half an infinite cylinder (e.g. $A$) is given by

$$\rho = U \sigma_A U^\dagger \sqrt{\sigma_B} \sigma_A U^\dagger,$$

(10)

with $\sigma_A$ the reduced density operators in $A$ for the virtual spaces across the bipartition, and $U$ an isometry. When the appropriate symmetries are present, as in the cases analyzed here, one has $\sigma_A = \sigma_B \equiv \sigma$, and therefore

$$\rho = U \sigma^2 U^\dagger.$$

(11)

Notice that this readily implies that $\rho$ and $\sigma^2$ are isospectral, since the isometries do not change non-zero eigenvalues, and therefore the Rényi entropies only depend on the eigenvalues of $\sigma$. And what is more: in terms of $\sigma$ the Rényi entropies now read

$$S^{(n)} = \frac{1}{1 - n} \log \left( \text{tr} (\sigma^{2n}) \right).$$

(12)

Thus, computing $S^{(n)}$ amounts to calculating $\sigma$, its powers, and its trace [16].

The calculation of $\sigma$ on an infinite cylinder for a 2d PEPS is a well-posed tensor network problem, since $\sigma$ is nothing but the dominant (left or right) eigenvector of the PEPS transfer matrix $T$, see Fig.14(b). This can be solved using many different strategies. Here we choose a similar approach to the one described in the main text for the GE: we compute this dominant eigenvector using the iTEBD method for non-unitary evolutions [1, 2]. The resulting dominant eigenvector can be written as an MPO of bond dimension $\chi$, which is then wrapped around a circle of length $L$, and constitutes our approximated $\sigma$. The computational cost of this calculation is $O(\chi^3 D^6)$ [15].

Next, by combining the obtained MPO for $\sigma$ with Eq.12 it is easy to see that, again, the calculation of any Rényi entropy $S^{(n)}$ can be reduced to some standard tensor network problem, see Figs.15 and 16. From here, the calculation strategy differs depending on whether we are interested in finite-$n$, or in the limit $n \to \infty$. The details of both cases are as follows:

**Finite-$n$ Rényi entropies**

In this case the calculation amounts to computing the tensor network contraction from Fig.15, taking into account the normalization of $\sigma^2$. Formally, the numerator inside the logarithm amounts to the contraction of a 2d tensor network on a torus of size $n \times L$, thus being quite similar to some of the contractions that were involved in the calculation of the GE in the main text. Therefore, we simply use now the same approach that was used there, i.e., we approximate the repeated multiplication of MPOs using iTEBD as explained in the first section of this supplementary material. After exactly $2n$ iterations we stop, and wrap the resulting MPO with bond dimension $\chi'$ around a circle of size $L$. The total computation time for this approach scales as $O(2n(\chi^2 \chi'^2 D^3 + \chi^3 \chi'^3 D^2) + L \chi'^3)$.
The case \( n = \infty \) deserves special attention. In principle, it should be possible to use the same trick as for finite-\( n \) above, taking the limit of a very large \( n \) until some convergence is reached. However, even if correct, such an approach is not necessarily the most efficient one. To understand this, simply notice that the largest eigenvalue \( \nu_1 \) of \( \rho \) also corresponds to the largest (normalized) eigenvalue of \( \sigma^2 \), i.e.,

\[
\nu_1 = \frac{v_L^T \sigma^2 v_R}{v_L^T v_R},
\]

(13)

with \( v_L \) and \( v_R \) respectively the left and right dominant eigenvectors of \( \sigma \). Since \( \sigma \) is given in the form of an MPO with periodic boundary conditions, it turns out that finding such dominant eigenvectors is also a standard 2d tensor network problem which we solve as done many times before: using iTEBD and wrapping the resulting MPS for \( v_L \) and \( v_R \), with bond dimension \( \chi' \), around a circle of size \( L \). In the end, \( S(\infty) \) is computed as in the diagram in Fig.16. The overall computational cost of this approach is \( O(\chi^3 \chi'^3 D^3 + L \chi^5 \chi'^5 D) \).

Some remarks are in order. First, if we are interested in extracting the topological component, we just proceed by doing finite-size scaling with \( L \), fitting the results to a linear function, and extrapolating the result down to \( L \rightarrow 0 \), exactly as we did for the GE. Second, the calculations of Rényi entropies with 2d PEPS can of course be improved in accuracy, especially if the correlation length is large (e.g. close to criticality). However, the practical drop in efficiency is very significant. And what is more: the same improvements that can be applied to Rényi entropy calculations can also be used, if necessary, to improve the accuracy in computing the GE. Third, we have observed that the calculations of the \( n \)-th Rényi entropies are extremely sensitive to truncations in the associated bond dimensions, which becomes especially important when \( n \) gets ‘large’. In practice, this means that we have been unable to produce sensible results for the topological contribution of Rényi entropies for \( n > 3 \) (except for infinity) because we cannot reach sufficiently
large bond dimensions with our computing resources. This is to be contrasted with the remarkable robustness and accuracy of the GE, already for small bond dimensions. In other words: for a comparable value of bond dimensions and computation time, the topological GE outperforms in accuracy the topological Rényi entropies by far, especially close to a quantum critical point.

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