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Gapless Hamiltonians for the toric code using the PEPS formalism

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We study Hamiltonians which have Kitaev’s toric code as a ground state, and show how to construct a Hamiltonian which shares the ground space of the toric code, but which has gapless excitations with a continuous spectrum in the thermodynamic limit. Our construction is based on the framework of Projected Entangled Pair States (PEPS), and can be applied to a large class of two-dimensional systems to obtain gapless “uncle Hamiltonians”.

Introduction.—Since its introduction by Wen in the 80’s, topological order has become a central subject of research both in the condensed matter and quantum information communities. The toric code, a many-body spin state originally introduced by Kitaev in the context of topological quantum computing [1], represents a paradigmatic example of a state with topological order. It is the ground state of a local, frustration free Hamiltonian H_{TC} defined on a two-dimensional lattice, whose degeneracy depends on the topology of the space on which it is defined. This Hamiltonian is gapped, and it exhibits (abelian) anyonic excitations. The toric code also possesses long-range entanglement (i.e., it cannot be created by local unitary operations out of a product state), and its entanglement entropy contains a universal part which can serve as a signature of its topological properties. All these properties are robust against local perturbations [2, 3]. Apart from that, it can be considered as an error correcting code with non-local encoding but local syndroms, and might therefore be useful as a quantum memory or for fault tolerant quantum computing.

The toric code can also be efficiently described in the language of tensor networks. As other states with topological order, it is a Projected Entangled Pair State (PEPS) of very low bond dimension, $D = 2$ [4, 5]. PEPS generalize Matrix Product States (MPS) [6, 7] to spatial dimensions higher than one, obey the area law for the entanglement entropy, and are believed to efficiently represent the ground states of local spin and fermionic Hamiltonians in lattices [8, 9]. Conversely, for any PEPS one can construct a frustration free *parent Hamiltonian* for which it is the ground state [5], which allows us to relate a given exotic quantum many-body state to physical Hamiltonians. In fact, H_{TC} is exactly such a parent Hamiltonian for the toric code, and using this construction in the PEPS formalism, one can readily uncover some of its most distinct properties [10]. In the same way, one can build parent Hamiltonians for many other strongly correlated states, such as string-net models [11], the AKLT state [12], resonating valence bond states, and others. In most of these cases, the resulting Hamiltonians are gapped above the ground state space, which makes them robust against local perturbations [13].

In this paper, we introduce an alternative way to construct Hamiltonians corresponding to MPS and PEPS, which we

term *uncle Hamiltonians*. The uncle Hamiltonian differs significantly from the parent Hamiltonian. While both Hamiltonians share the same ground state subspace by construction, their spectra are extremely different: As we prove, the uncle Hamiltonian is gapless and has a continuous spectrum in the thermodynamic limit, which is in sharp contrast to the gapped parent Hamiltonian. Our construction exploits the fact that the link between tensor networks and their associated parent Hamiltonians is not robust under generic perturbations [14] for a large class of interesting MPS and PEPS, in particular for systems with symmetry breaking and topological order.

Our findings are interesting from several perspectives. First, they show that the association between PEPS and Hamiltonians is more ambiguous than generally believed. Second, it illustrates that care must be taken when trying to define topological order in terms of properties of the ground state alone, such as its topological entropy [15, 16], as the same quantum state can appear as a ground state of both a gapped (topological) and a gapless (unstable) Hamiltonian. Finally, it also provides a clear example of a gapless system which nevertheless does not exhibit any critical (or even finite-range) correlations.

Uncle Hamiltonian for the GHZ state.—We start by explaining our construction for the GHZ state in order to introduce the key concepts.

A state $|\psi\rangle \in (\mathbb{C}^d)^{\otimes L}$ is called a (translationally invariant) Matrix Product State (MPS) if it can be written as

$$|M(A)\rangle = \sum_{i_1, \dots, i_L} \text{tr}[A_{i_1} \cdots A_{i_L}] |i_1, \dots, i_L\rangle,$$

where the A_i are $D \times D$ matrices, D being called the *bond dimension*, L is the number of sites and d the physical dimension at each site. These matrices can be thought of as a tensor A with three indices $(A_i)_{\alpha\beta}$, two of them (α, β) being the matrix indices (“virtual indices”) and the third index (i) corresponding to the physical spin (“physical index”).

The unnormalized GHZ state on n particles can be expressed as an MPS as follows:

$$|\text{GHZ}\rangle = \sum_{i_1, \dots, i_n} \text{tr}[A_{i_1} \cdots A_{i_n}] |i_1 \dots i_n\rangle = |00 \dots 0\rangle + |11 \dots 1\rangle,$$

where $i_j \in \{0, 1\}$ and $A_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $A_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

A parent Hamiltonian $H = \sum_i h_{\text{loc}}$ of an MPS is obtained as a sum of local orthogonal projections $h_{\text{loc}} = h_{i-1, i, i+1}$ acting on three consecutive sites, each of them with kernel [7, 10].

$$\text{span} \left\{ \sum_{i_1 i_2 i_3} \langle i | A_{i_1} A_{i_2} A_{i_3} | j \rangle | i_1 i_2 i_3 \rangle, i, j \in \{0, 1\} \right\};$$

for the GHZ state, $\ker h_{\text{loc}} = \text{span}\{|000\rangle, |111\rangle\}$ [19]

The parent Hamiltonian H is frustration free since its ground space is the intersection of these kernels. The GHZ state lies in the ground space, which is 2-dimensional and is spanned by the states $|0\rangle^{\otimes n}$ and $|1\rangle^{\otimes n}$, and the Hamiltonian has an spectral gap between the ground space and the rest of energy levels.

Let us now perturb the GHZ state in the MPS representation, by considering small random linear perturbations of the matrices A_i ,

$$A_0^\varepsilon = A_0 + \varepsilon \begin{pmatrix} a_0 & b_0 \\ c_0 & d_0 \end{pmatrix}, A_1^\varepsilon = A_1 + \varepsilon \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix}.$$

The parent Hamiltonian H^ε corresponding to this new MPS is the sum of a new local projector $h_{\text{loc}}^\varepsilon$ with

$$\ker h_{\text{loc}}^\varepsilon = \text{span} \left\{ \sum_{i_1 i_2 i_3} \langle i | A_{i_1}^\varepsilon A_{i_2}^\varepsilon A_{i_3}^\varepsilon | j \rangle | i_1 i_2 i_3 \rangle, i, j \in \{0, 1\} \right\}.$$

This kernel is spanned by the vectors

$$\begin{aligned} & |000\rangle + O(\varepsilon), \\ & |111\rangle + O(\varepsilon), \\ & \varepsilon [b_0 |000\rangle + (b_0 + b_1)(|001\rangle + |011\rangle) + b_1 |111\rangle] + O(\varepsilon^2), \\ & \varepsilon [c_0 |000\rangle + (c_0 + c_1)(|100\rangle + |110\rangle) + c_1 |111\rangle] + O(\varepsilon^2), \end{aligned}$$

or equivalently by the vectors

$$\begin{aligned} & |000\rangle + O(\varepsilon), \quad |0+1\rangle + O(\varepsilon), \\ & |111\rangle + O(\varepsilon), \quad |1+0\rangle + O(\varepsilon), \end{aligned}$$

as long as $b_0 + b_1 \neq 0$ and $c_0 + c_1 \neq 0$, which holds for almost every perturbation. $[|0+1\rangle$ denotes $|0\rangle|+\rangle|1\rangle$, etc., where $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$

As we let ε tend to 0, this local projector does not converge to the original $h_{i-1, i, i+1}$. Instead, it converges to a projector with kernel $\text{span}\{|000\rangle, |0+1\rangle, |1+0\rangle, |111\rangle\}$, which we denote by $h'_{\text{loc}} = h'_{i-1, i, i+1}$ for the corresponding sites. The resulting global Hamiltonian $H' = \sum_i h'_{i-1, i, i+1}$ is the one we will call the *uncle Hamiltonian*. As $\ker h_{\text{loc}} \subset \ker h'_{\text{loc}}$, H' has all the ground states of H and is thus frustration free. On the other hand, the presence of the vector $|0+1\rangle$ in the ground state subspace also allows for zero-momentum superpositions of “domain walls” between domains of 0’s and 1’s, $\dots + |\dots 001 \dots\rangle + |\dots 011 \dots\rangle + \dots$, and correspondingly for $|1+0\rangle$. However, it is easy to see that these configurations cannot exist in the ground space given periodic boundary conditions[20], and thus, the ground state subspace for

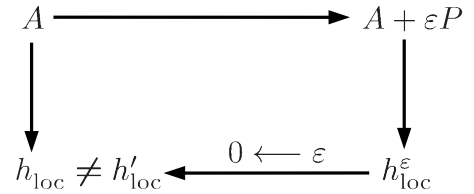


FIG. 1: Construction of the uncle Hamiltonian. Any MPS and PEPS tensor A induces a corresponding parent Hamiltonian h_{loc} . The *uncle Hamiltonian* is constructed by perturbing $A \rightarrow A + \varepsilon P$, computing its parent Hamiltonian $h_{\text{loc}}^\varepsilon$, and finally taking ε to zero. As we show, the resulting uncle Hamiltonian $h'_{\text{loc}} = \lim h_{\text{loc}}^\varepsilon$ can be very different from the parent Hamiltonian h_{loc} .

H' is the same as for the parent Hamiltonian H . On the other hand, H' is gapless in the thermodynamic limit, and moreover, its spectrum is the whole positive real line \mathbb{R}^+ . This can be proven utilizing the “domain wall superpositions” mentioned above, by using the unnormalized states

$$|\varphi_{r,A}\rangle = \sum_{\substack{1 \leq i < j \leq A, \\ 2 \leq j-i \leq r}} |\dots 0\rangle |0^1 0 \dots 0^i 1 1 \dots 1^j 0 \dots 0^A\rangle |0 \dots\rangle, \quad (1)$$

where the superscripts indicate the position of the corresponding site. The $|\varphi_{r,A}\rangle$ are orthogonal to the ground space and have energy as close to $C/(r-1)$ as desired if we allow both the chain length and A grow, for some given constant C and any r , which implies the existence of low eigenvalues tending to 0. The locality of the uncle Hamiltonian renders it possible to concatenate approximate eigenvectors in the thermodynamic limit and therefore to conclude that the sum of two elements in the spectrum is also in the spectrum, which finally allows to prove that the spectrum of H' becomes continuous in the thermodynamic limit, $\sigma(H') = \mathbb{R}^+$. Moreover, the spectra of H' acting on finite size chains tend to be dense on the positive real line as the size of the chain grows. A detailed analysis is given in Ref. [17], where it is also shown that in one dimension, this behavior occurs for any MPS with degenerate parent Hamiltonian (i.e., non-injective MPS). In contrast, for systems with unique ground states (i.e., injective MPS) the parent Hamiltonian is robust under perturbations. However, one can still construct gapless uncle Hamiltonians by taking non-injective MPS representations of these states, but in this case the similarities between parent and uncle Hamiltonians are weaker [17].

The toric code as a PEPS.—Projected Entangled Pair States (PEPS) are the natural generalization of MPS to general lattices. For simplicity, we restrict to square lattices. Then, the three-index tensors A have to be replaced by five-index tensors, with four virtual indices and one physical index. The virtual indices of each tensor are contracted with the corresponding indices of the adjacent tensors as depicted in Fig. 2, where connected lines denote the contraction of indices. The physical index will be denoted by a black dot in the upper left corner of each tensor, and should be thought of as a tensor leg pointing out of the paper.

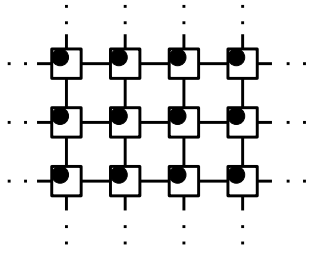


FIG. 2: Graphical description of PEPS.

Under certain conditions on the tensors [10], a parent Hamiltonian can be constructed by considering local projections h_{loc} for every 2×2 region onto the orthogonal complement of the space

$$\ker h_{\text{loc}} = \left\{ \begin{array}{|c|c|} \hline \bullet & \bullet \\ \hline \text{A} & \text{B} \\ \hline \bullet & \bullet \\ \hline \text{C} & \text{D} \\ \hline \end{array} , b \text{ boundary tensor} \right\} \quad (2)$$

(spanned by all the possible boundary tensors b), and summing these local projectors to construct a global Hamiltonian. The ground space of this parent Hamiltonian is the intersection of the kernels of the local projectors.

A PEPS representation of the toric code can be obtained by considering a PEPS with bond dimension two, and associating the virtual space with the physical space at every site, $\mathbb{C}^d = (\mathbb{C}^2)^{\otimes 4}$. The tensor E at every site is then the orthogonal projection onto the space of spin configurations with even parity in the virtual space, $E|ijkl\rangle = (1 + (-1)^{i+j+k+l})|ijkl\rangle/2$.

The ground space of the parent Hamiltonian for this PEPS is locally equivalent to the toric code. A detailed treatment of this relationship can be found in [10].

Uncle Hamiltonian for the toric code.—Let us now derive the uncle Hamiltonian for the toric code. This will be done as for the GHZ state, cf. Fig. 1: We perturb the toric code tensors, derive the corresponding parent Hamiltonian, and take the limit of vanishing perturbations. The specific perturbation we consider, which we denote by O , is the projection complementary to E , $O = \mathbb{I} - E$, the projection onto the space of odd spin configurations.

The 2×2 -site local Hamiltonian $h_{\text{loc}}^\varepsilon$ is obtained from Eq. (2) by letting each of the four tensors be $E + \varepsilon O$. In the limit $\varepsilon \rightarrow 0$, we obtain a new projector $h'_{\text{loc}} = \lim h_{\text{loc}}^\varepsilon$ different from the local projector h_{loc} we started with: The new local Hamiltonian h'_{loc} is the projector onto the orthogonal complement of $E_{22} + O_{22} = \ker h'_{\text{loc}}$, where

$$O_{22} = \left\{ \sum_{\text{pos } O} \begin{array}{|c|c|} \hline \bullet & \bullet \\ \hline \text{O} & \text{E} \\ \hline \bullet & \bullet \\ \hline \text{E} & \text{E} \\ \hline \end{array} , b \text{ boundary tensor} \right\}, \quad (3)$$

and the sum runs over the positions which the single O tensor above may occupy among the four tensors appearing. E_{22}

is defined analogously, but contains only E tensors. Note that E_{22} will only be non-vanishing for even parity boundary conditions b , whereas for O_{22} this will only be the case for odd boundary conditions. The space E_{22} plays the role $\text{span}\{|000\rangle, |111\rangle\}$ did in the uncle Hamiltonian of the GHZ state, and O_{22} plays the role of $\text{span}\{|0+1\rangle, |1+0\rangle\}$. Intuitively, while E_{22} only supports states without anyonic excitations, O_{22} allows for configurations with exactly one anyon which is distributed in a uniform superposition. As with the domain walls in 1D, the idea is that such configurations cannot appear in the ground state subspace as anyons come in pairs, but two excitations are not allowed to meet; however, such configurations with delocalized anyon pairs will have low energy.

The new uncle Hamiltonian H' is constructed again as the sum over all 2×2 regions of the local projector h'_{loc} . When considering an $n \times m$ contractible region R , and the sum of the local projectors acting entirely in this region, one finds that the kernel of this sum has the same structure as the kernel of a single projector:

$$\ker \left(\sum_R h'_{\text{loc}} \right) = \bigcap_R \ker h'_{\text{loc}} = E_{nm} + O_{nm},$$

with definitions for E_{nm} and O_{nm} similar to Eq. (3); the detailed proof is given in Appendix A. However, the O subspace vanishes when considering the whole lattice and imposing periodic boundary conditions, as those are automatically even (see Appendix A). Therefore, the global ground space of the new Hamiltonian is the same as the ground space of the toric code parent Hamiltonian.

Spectrum of the uncle Hamiltonian.—Let us now show that the uncle Hamiltonian for the toric code is gapless with continuous spectrum in the thermodynamic limit. As we did with the GHZ uncle Hamiltonian, we will consider a family of low energy states which are orthogonal to the ground space. Given any integer value of r , we may take two contractible rectangles R_1 and R_2 of size $r \times r$ which are separated by at least two sites. We construct a family of unnormalized states $|\phi_r\rangle$ by placing at these two regions the tensor O_{rr} [cf. Eq. (3)], and setting all remaining tensors to E :

$$|\phi_r\rangle = \sum_{\substack{\text{pos } \\ O_1 \in R_1 \\ \text{pos } \\ O_2 \in R_2}} \begin{array}{|c|c|c|c|c|c|} \hline \text{E} & \text{E} & \text{E} & \text{E} & \text{E} & \text{E} \\ \hline \text{E} & \text{E} & \text{E} & \text{E} & \text{E} & \text{E} \\ \hline \text{E} & \text{E} & \text{E} & \text{E} & \text{E} & \text{E} \\ \hline \text{E} & \text{E} & \text{E} & \text{E} & \text{E} & \text{E} \\ \hline \text{E} & \text{E} & \text{E} & \text{E} & \text{E} & \text{E} \\ \hline \text{E} & \text{E} & \text{E} & \text{E} & \text{E} & \text{E} \\ \hline \end{array}. \quad (4)$$

This is, each of the gray regions contains exactly one O tensor and E 's otherwise, and the sum runs over the position of the two O 's.

The norm of all these summands is the same, say C . This value depends only on the total dimension of the lattice. The norm of any of these $|\phi_r\rangle$ is Cr^2 (since the summands are mutually orthogonal and there are r^4 of them), but only the h'_{loc} which overlap with the boundary of these regions contribute a positive energy. There are only $8r$ of them, $4r$ acting on the left and $4r$ acting on the right region. For each of

them at most $2r^2$ summands from (4) add any energy: there are at most two ways O can overlap with the Hamiltonian term, and the r^2 comes from the O in the other region. Hence $\langle \phi_r | H' | \phi_r \rangle \leq C^2 O(r^3)$, and the energy $\langle \phi_r | H' | \phi_r \rangle / \langle \phi_r | \phi_r \rangle$ of these states decreases as $O(1/r)$. Altogether, this proves that H' is gapless.

In order to prove that the spectra of these Hamiltonians tend to become dense in the positive real line \mathbb{R}^+ , we fix one of the dimensions of the system—let us choose the vertical one—and let the other go to infinity. This results in an MPS-like problem, in which we can take the thermodynamic limit.

Since the vertical dimension is fixed – let us say its value is N – the regions used to construct the states $|\phi_r\rangle$ from (4) cannot grow indefinitely. We can consider instead similar unnormalized states $|\phi_{r,N}\rangle$, coming from $r \times N$ regions, to prove the existence of a suitable set of elements in the spectrum $\{\lambda_i\}$ tending to 0, from which it can be shown that any finite sum of these values also lies in the spectrum. These finite sums are dense in $[0, \infty)$, which therefore coincides with the spectrum due to its necessary closedness.

The same values $\sum \lambda_i$ lie close to eigenvalues of the uncle Hamiltonian for some finite sized –but big enough– lattices. Hence the spectra of the finite sized uncle Hamiltonians tend to be dense in $[0, \infty)$.

The analogue proof for the uncle Hamiltonian of the GHZ is detailed in [17], and a sketch of the steps adapted to the toric code can be found in Appendix B.

Conclusions.—In this paper, we have used the framework of PEPS to study different ways in which strongly correlated quantum systems can appear as ground states of local Hamiltonians. In particular, we have introduced the *uncle Hamiltonian* of a PEPS, which contrasts with the usually considered parent Hamiltonian. The uncle Hamiltonian is obtained by perturbing the PEPS tensors, computing the corresponding parent Hamiltonian, and then taking the perturbation to zero. As parent Hamiltonians of systems with degenerate ground states are not robust under perturbations of the tensors, the resulting uncle Hamiltonian behaves very different from the parent Hamiltonian: While the parent and the uncle Hamiltonian share the same ground state space, the uncle is gapless with a continuous spectrum in the thermodynamic limit, thus behaving very differently. We have demonstrated our approach with Kitaev’s toric code: The resulting uncle Hamiltonian has the toric code state as its ground state, however, it is gapless and thus does not yield a topologically protected system. This both demonstrates the ambiguity in the association of PEPS with local Hamiltonians, and the subtleties one has to take care of when identifying topological order from the ground state rather than the properties of the interaction.

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 - [20] For periodic boundary conditions, domain walls come in pairs, i.e., for every $|0+1\rangle$ (“up”) domain wall there is a $|1+0\rangle$ (“down”) domain wall. Since both domain walls are in a momentum eigenstate, there is a non-zero probability that they are at adjacent sites, leading to a configuration $|010\rangle$ which is penalized by the Hamiltonian.