Projected entangled pair states (PEPS) have emerged as a central notion in our understanding of quantum many-body systems on a lattice [1]. On the numerical front, these states support non-perturbative approaches to glean information about the ground state of challenging Hamiltonians such as the $t-J$ or the Heisenberg models [2, 3]. On the theoretical front, PEPS provide a framework to systematically investigate various phases of matter, such as symmetry protected phases, or intrinsic topological phases [4]. The power of PEPS resides in their ability to represent area laws for entanglement, and in their compact description, where all the information about the quantum state is encoded in a set of local tensors associated each with a site of the lattice.

However, a formidable difficulty arises when one attempts to actually use these states. Generically, evaluating mean values of physical observables turns out to be a #P-hard problem, and a black box that prepares PEPS would allow to solve PP problems [4]. In this landscape, it is legitimate to look at the complexity of a simpler question: what is the complexity of deciding whether a given tensor network state is naught? For general tensor network states, this problem has been proven to be NP-hard [2].

In this paper, we will show that NP-hardness persists if we restrict to PEPS. As we will see, specialising the no-go result of Ref. [7] allows to reveal limitations of the PEPS framework which, to the best of our knowledge, were unknown so far. First, we will see that the result can be somewhat pushed further: we will exhibit a class of PEPS for which the problem of zero testing is actually undecidable. Next, we will turn to corollaries of these impossibility results that are relevant to the general program of using PEPS to describe strongly correlated quantum systems. No PEPS analogue of the fundamental theorem for matrix product states exists; it is NP-hard/undecidable to say whether the state associated with a given tensor possesses a certain symmetry or not; determining whether the parent Hamiltonian of a PEPS is gapped is undecidable. As a by-product, we observe that the 2-local commuting hamiltonian problem (2-CLH), with nearest-neighbour interactions, and bulk translational invariance, contains an NP-complete sub-family of instances. The key ingredient of the present study is a simple encoding of tiling problems into a PEPS.

We start with the basic definitions. Consider a set of $n$ identical ‘spin’ particles on a line, each with a local dimension $d$. An MPS is a state of the form

$$|\psi\rangle = \sum_{s_1=1}^{d} \cdots \sum_{s_n=1}^{d} A_1(s_1) \cdots A_n(s_n) |s_1 \cdots s_n\rangle,$$

where each $A_k(s)$ is a matrix. Namely, all $A_k(s)$ have a fixed size $D \times D$ for $k = 2 \ldots n - 1$, while the matrices $A_1(s)$ have dimensions $1 \times D$, and the matrices $A_n(s)$ have dimensions $D \times 1$ (open boundary conditions assumed). It has been proven that the ground states of one-dimensional gapped quantum systems are well represented by MPS whose bond dimension $D$ does not depend on $n$ [4-11]. One can observe that the number of parameters necessary to specify an MPS, $ndD^2$ complex numbers, only grows linearly with $n$, whereas the dimension of the full Hilbert space where it lives grows exponentially with $n$. The higher $D$, the more entanglement can be represented. MPS allow for a diagrammatic description specified by two rules: (i) a tensor is represented by a vertex with a number of legs sticking out equal to the number of indices of the tensor, (ii) summation over repeated indices amounts to gluing legs. With these two rules, Eq. (1) is equivalent to Fig. 1.

A PEPS is a two-dimensional generalisation of Fig. 1.
The Bounded tiling is where

Theorem 1. Given a boundary condition, a tiling is any assignment of a colour with each link of the boundary, and a tiling is a set of colours, a boundary condition, a tile set, and if the boundary condition is respected. The tuple of colours around each plaquette belongs to the a finite set of colours $\Gamma$, a tile set, and if the boundary condition is respected. The tuple of colours around each plaquette belongs to the $\Gamma$. Considering a square lattice $\Lambda$ where four colour degrees of freedom $(u, d, l, r)$ live at the centre of each plaquette. The energy operator is

$$H^{BT} = \sum_{(p,p')} h^T_{p,p'} + \sum_{p \in \partial \Lambda} h^\partial_{p}.$$  

The bulk contribution to $H^{BT}$ encodes the constraints that (i) each bulk plaquette should be in a state that corresponds to an element of $T$, (ii) two adjacent plaquettes should have the same colour on their common edge. For example, if two plaquettes $p, p'$ meet on a vertical edge,

$$h^T_{p,p'} = 1^{\otimes 8} - \sum_{w, w' \in T} \delta(w_l,w'_l) \langle w, w' | w, w' \rangle.$$  

Regarding the boundary contribution, if $p$ denotes e.g. a plaquette located on the top edge of the lattice, we want the state of $p$ to be in correspondence with an element of $T$ such that the top colour has some value $\gamma_p$. This requirement can be enforced with

$$h^\partial_p = 1^{\otimes 4} - \sum_{w \in T} \delta(w_u, \gamma_p) \langle w \rangle.$$  

It is obvious that $H^{BT} \geq 0$ and that the ground state energy of $H^{BT}$ is zero if and only if the associated BT problem admits a solution. This observation allows to relate the BT problem with the $k$-local Hamiltonian problem. In the latter, the input is a Hamiltonian $H$ and two real parameters $\alpha, \beta$. The Hamiltonian acts on $n$ qudits and is a sum of $k$-body terms; $\alpha$ and $\beta$ satisfy $\alpha - \beta \geq 1/\text{poly}(n)$. The task is to decide whether the ground state energy of $H$ is at most $\alpha$ or at least $\beta$. What makes this problem interesting is its computational power. For instance, quantum 2-local Hamiltonian is QMA-complete [14]. Versions of the problem where all the terms appearing in the Hamiltonian commute (CLH) are computationally interesting too. For instance, there is a variant of a problem involving qubit plaquette interactions which is in NP [16]. For more results on the CLH problem, see [15]. The Hamiltonian $H^{CLH}$ associated with BT allows to make an observation along these lines. We get the following result.

Theorem 2. The 2-CLH problem, with $\alpha = 2\beta = 2/3$, and with $H$ defined as in (2) is NP-complete.

Note that such hardness results also follow e.g. from Barahona’s results that finding the ground state energy of a bilayer spin glass is NP-hard [17]. However, our construction shows NP-completeness for a Hamiltonian that is translationally invariant in its bulk.

We now turn back to the main issue of this paper, and consider a square lattice where four colour degrees of freedom $(u, d, l, r)$ live at the centre of each plaquette. The energy operator is

$$A^{(w)}_T(s) = \sum_{w' \in T} \delta(w, w') \delta(w, s).$$  

![Diagram](image_url)  

Figure 1. Diagrammatic representation of an MPS.

![Diagram](image_url)  

Figure 2. Diagrammatic representation of a 4 × 5 PEPS. The diagonal legs represent physical degrees of freedom, whereas horizontal and vertical legs represent virtual degrees of freedom.
On a top edge plaquette with colour set to some value \( \gamma \),
\[
A_{\text{top}}(\gamma,w_1,w_2,w_3) \sum_{w' \in T} \delta(\{\gamma, w_1, w_2, w_3\},w') \delta(w',s).
\]

The tensors are given by similar expressions for the three other edges and for the four corners. Since tensors on neighbouring sites are patched by identifying left/right or up/down virtual indices, we see that the solutions of adjacent plaquettes should match, and comply the boundary condition. Therefore, \( |\Phi_{\text{BT}}]\neq 0 \) if and only if \( \Phi_{\text{BT}} \) admits a non-zero ground state of \( H_{\text{BT}} \). This observation, combined with Theorem 1, proves the following:

**Theorem 3. PEPS zero testing is NP-hard.**

An alternative way to understand the proof of the Theorem is to note that projections onto zero-energy spaces of commuting Hamiltonians, including NP-hard ones, and thus the equal weight superposition of all zero-energy configurations, are PEPS [5]; in fact, this is exactly what the PEPS construction above achieves for the Hamiltonian [3].

It is well known that there is no algorithm, however inefficient, that can determine whether there exists a periodic tiling of the plane with \( T \) the problem is algorithmically undecidable (see Appendix B). As in the above case where there is a boundary, we can associate a PEPS with the problem of tiling the plane periodically or, equivalently, an \( \ell_x \times \ell_y \) torus. This state is obtained by patching the tensor \( T \) \( \ell_x \times \ell_y \) times, with periodic identification. This PEPS is non-zero if and only if a tiling of the plane with periods \( \ell_x, \ell_y \) exists. We conclude the following.

**Theorem 4. There is no algorithm that receives a PEPS tensor on input, and correctly decides whether the associated state is naught on all \( \ell_x \times \ell_y \) tori.**

**N.B.** The relation between algorithmic and axiomatic undecidability implies that there exists infinitely many PEPS tensors for which determining whether the corresponding PEPS is naught on all \( \ell_x \times \ell_y \) torus cannot be decided, starting from any recursive and consistent set of mathematical axioms.

In the rest of the paper, we discuss three implications of our findings. A first implication is concerned with symmetries. Let \( |\Phi_T\rangle \) denote the state resulting from patching the tensor \( T \) around a torus, and consider \( |\Phi\rangle = |\Phi_S\rangle + |\Phi_T\rangle \), where \( |\Phi_S\rangle \) denotes a state invariant under some symmetry that \( |\Phi_T\rangle \) lacks. \( |\Phi\rangle \) admits a PEPS description where the local tensor is the direct sum of the local tensors for \( |\Phi_S\rangle \) and \( |\Phi_T\rangle \). We see that we can claim that \( |\Phi\rangle \) has the symmetry iff we can determine whether \( |\Phi_T\rangle = 0 \). Therefore, there cannot be a necessary and sufficient algorithmically decidable condition for a PEPS to have a symmetry; this situation sharply contrasts with the one-dimensional case [22].

In one spatial dimension, a key ingredient that has enabled our current understanding of phases of matter describable by matrix product states is the existence of a so-called fundamental theorem [20] that relates global and local descriptions. In substance, this theorem states if two sets of tensors \( \{A_k : k = 1 \ldots n\} \) and \( \{A_k' : k = 1 \ldots n\} \) give rise to the same tensor, the identity is reflected at the tensor level. If, say, we consider a transitionally invariant spin chain, there exists a universal operation \( f \) (canonical form framing) and a local specific operation (similarity transformation) \( T \) such that

\[
T(f(A_k)) = f(A_k').
\]

**Theorem 4** is an obstruction to a PEPS analogue of this construction. For example, on the plane, such a theorem would allow to decide on the equivalence between the zero state, certainly represented by the null tensor, and the PEPS represented by the tensor \( A \). Therefore, one of \( f \) or \( T \) either does not exist or is uncomputable. It is natural to wonder what happens when the states are guaranteed to be non-zero. Could it be the case that a fundamental theorem then becomes possible? The above discussion on symmetries provides a negative answer. Pick \( |\Phi_S\rangle \neq 0 \): a fundamental theorem would allow to decide whether \( |\Phi_S\rangle = |\Phi_S\rangle + |\Phi_T\rangle \).

Our third implication is concerned with spectral properties. The undecidability of the spectral gap for short-range Hamiltonians has been established in [3]. We now show that even if we restrict to Hamiltonians that are parent Hamiltonians of a PEPS, undecidability still holds, at least in the case of a finite but unbounded local physical dimension. For that purpose, let us recall a standard procedure to associate a nearest neighbour parent Hamiltonian with a PEPS described by a tensor \( A \) [21]. With any region \( R \) of the lattice, we associate a linear map

\[
\chi(A,R) : (\mathbb{C}^D)^{\otimes |IR|} \rightarrow (\mathbb{C}^D)^{\otimes |IR|} : |C\rangle \rightarrow \sum_{i \in R} C[A_{ih}C]|i_R\rangle.
\]

A parent Hamiltonian is any nearest neighbour Hamiltonian \( H = \sum_{p,p'} h_{p,p'} \sum_{i \in R} C[A_{ih}C]|i_R\rangle \).

Such a construction for the tensor \( A \) yields a parent Hamiltonian \( H_T = \sum_{p,p'} h_{p,p'} \) such that \( h_{p,p'} \leq 0 \), and such that

\[
\ker h_{p,p'} = \text{Im } \chi(A_T,p \cup p').
\]

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\[
\ker h_{p,p'} = \text{Im } \chi(A_T,p \cup p').
\]
For this system, we will be interested in the state
\[ |\Psi\rangle = |\Psi_G\rangle + |\Psi_Z\rangle \otimes |\Psi_T\rangle, \]
where \(|\Psi_G\rangle\) is a PEPS living in \(\mathcal{H}_1^{\otimes n}\), and where \(|\Psi_Z\rangle\) is a PEPS living in \(\mathcal{H}_2^{\otimes n}\). \(|\Psi\rangle\) is clearly a PEPS: its local tensor is given by
\[ A = A_G \oplus (A_Z \otimes A_T). \] (6)

One easily proves the identity
\[ \text{Im} \chi(A, R) = \text{Im} \chi(A_G, R) \oplus \{\text{Im} \chi(A_Z, R) \otimes \text{Im} \chi(A_{BT}, R)\} \]
for any region \(R\). To make our point, it will be enough that \(\mathcal{H}_1\) be one-dimensional, and its (unique) basis state will be denoted by \(|0\rangle\). We will also choose \(|\Psi_G\rangle\) to be such that its parent Hamiltonian is gapless and has \(|\Psi_Z\rangle\) as unique ground state, e.g. the Ising PEPS discussed in [5].

Thus, \(|\Psi\rangle\) is a Hamiltonian described by the two-body interaction
\[ h_{pp'} = |0\rangle\langle 0|_p \otimes 1^Z_{p'} + 1^Z_p \otimes |0\rangle\langle 0|_p' \]
\[ + h^Z_{pp'} \otimes 1^{T}_{p'} + 1^{Z}_{pp'} \otimes h'^{Z}_{pp'}. \] (7)
h_{pp'} is evidently a semi-definite positive operator. In order to prove that \(H = \sum_{(p,p')} h_{pp'}\) is a parent Hamiltonian for \(|\Psi\rangle\), we prove that \(\ker h_{pp'} \subseteq \text{Im} \chi(A, p \cup p')\).

Consider then some state \(|\phi\rangle \in \ker h_{pp'}\). The first two penalty terms imply that \(|\phi\rangle = |00\rangle_{pp'} + |\phi_{ZT}\rangle_{pp'}\), where \(|\phi_{ZT}\rangle_{pp'} \in (\mathcal{H}_2 \otimes \mathcal{H}_T)^{\otimes 2}\). Clearly, \(|00\rangle_{pp'} \in \text{Im} \chi(A_G, p \cup p')\) and \(|00\rangle_{pp'} \in \ker h_{pp'}\). Therefore \(|\phi\rangle \in \ker h_{pp'}\) if and only if \(|\phi_{ZT}\rangle \in \ker h_{pp'}\). This latter condition can only be met if \(h^Z_{pp'} \otimes 1^{T}_{p'}|\phi_{ZT}\rangle = 0\), and if \(1^{Z}_{pp'} \otimes h'^{Z}_{pp'}|\phi_{ZT}\rangle = 0\). That is,
\[ |\phi_{ZT}\rangle = \{\text{Im} \chi(A, p \cup p') \otimes H^Z_{pp'}\} \cap \{\text{Im} \chi(A_T, p \cup p')\} \]
\[ = \text{Im} \chi(A, p \cup p') \otimes \text{Im} \chi(A_T, p \cup p'). \]

Thus, \(|\phi\rangle \in \text{Im} \chi(A, p \cup p')\). The inclusion \(\ker h_{pp'} \supseteq \text{Im} \chi(A, p \cup p')\) is proven likewise. Using the property that \(h'_{pp'} \geq h^T_{pp'}\) allows to recycle the argument exposed in Theorem 7 of Section 5.1 of [8], and prove:

**Theorem 5.** There is no algorithm that receives on input the tensor of a PEPS, \(A\), together with the description of a nearest-neighbour parent Hamiltonian for \(A\), and correctly decides whether the latter is gapped in the thermodynamic limit.

Note that if a nearest-neighbour parent Hamiltonian of a PEPS is gapped, then all of them are. Hence, in the above theorem, one can always take as a parent Hamiltonian the one where \(h_{pp'}\) is the projector onto \((\text{Im} \chi(A, p \cup p'))^\perp\).

In summary, we have analysed the issue of PEPS zero testing. Depending on details that specify the problem, we have found it to be NP-hard or undecidable. These results have allowed us to reveal obstructions regarding the existence of a fundamental theorem for PEPS, or the local characterisation of a symmetric PEPS. We have also revisited the undecidability of the spectral gap for short-range Hamiltonians, and shown it to hold even for Hamiltonians that are parent of a PEPS. Perhaps the main conclusion to be drawn from these findings is that, despite its appealing simplicity, the PEPS framework, without additional assumptions, is too broad to work with. Actually, to the best of our knowledge, all the situations where these obstructions are overcome involve some additional assumption; typically a form of injectivity [23]. We believe our results invite to a systematic investigation of conditions that turn the PEPS formalism tractable and are physically sound.

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Appendix A: Turing machines and bounded tilings

In this Appendix we define the Bounded Tiling (BT) problem and show its NP-completeness. We start with the necessary definitions.  

A Turing Machine (TM) is defined by the following data:

- A 2-way infinite tape, seen as an array of cells,
- A head, which can read and write from the tape,
- A finite set Σ of symbols of the tape cells (alphabet),
- A finite set K of states of the head,
- A register that keeps track of the current state of the head,
- A program, i.e., a finite table of instructions represented by quintuples (q, s, q', s', M) ∈ K × Σ × K × Σ × {Left, Stay, Right}.

The set Σ includes a special blank symbol #, and the set K includes the initial state q0 and the final accepting state qF.

The machine is initialised by writing an input (a non-blank sequence of symbols from Σ) on the tape, positioning the head to the leftmost symbol of the input, and preparing it in the state q0. A computation, then, is a sequence of actions each governed by some quintuple of the program as follows: If the register contains the state q and the head reads on the tape the symbol s, a quintuple of the form (q, s, q', s', M) is selected. On instruction (q, s, q', s', M) the register is updated to q', the symbol s' is written on the tape and the head is moved in the direction given by M. The Turing machine halts when no suitable instruction exists to continue, and it accepts the input when it halts with the state qF written in the register. (One can always modify a machine so that halting and accepting coincide, i.e., it halts if and only if it accepts.)

A TM is deterministic if for each pair (q, s) ∈ K × Σ there is at most one instruction of the form (q, s, ..., ) in the program, and it is non-deterministic otherwise. A non-deterministic machine accepts an input if there exists some computation leading to the state qF.

An instantaneous description (ID) of a TM is a specification of the current symbols written on the tape, and the position and state of the head. An example is the following:

\[ \ldots, \#, \#, s_1, s_2, s_3, q, s_4, s_5, \#, \#, \ldots \]

which is a way to represent a machine with the head in state q pointing at the fourth cell, and reading s4. As another example, after instruction (q, s4, q', s', L) the ID is

\[ \ldots, \#, \#, s_1, s_2, q', s_3, s', s_5, \#, \#, \ldots \]

One can represent a t-step computation with a sequence of IDs T0, T1, ..., Tt so that each step Ti, Ti+1 is consistent with some instruction from the program. Then, a machine accepts an input w if and only if there is a sequence of IDs where T0 = ..., #, q0, w, #, ... and Tt = ..., #, qF, w, #, ... We then say that there exists an accepting computation for w with this TM.

Turing showed in his seminal paper that there are universal Turing Machines (UTMs): machines that can simulate with polynomial overhead any other machine by accepting its description as part of the input. In other words, for every machine T (described by a bitstring t) on input x, the universal TM U satisfies

\[ U(t, x) = T(x), \]

and if computing \( T(x) \) takes \( t \) steps, computing \( U(t, x) \) takes \( poly(t) \) steps. One interesting aspect of these universal TMs is that their programs can be quite short. For instance, there exists a UTM with \( |K| = 5 \) and \( |Σ| = 7 \), which means that the program contains at most \( 3|K|^2|Σ|^2 = 3675 \) instructions.

A language is any subset of the set of all possible sequences of Σ symbols: \( Σ^* \). A simple example of a language is the set of all even natural numbers in binary representation. A TM accepts a language L, if for any \( w \in Σ^* \), there exists an accepting computation if \( w \in L \).

Languages can be arranged in complexity classes, according to the resources needed by a TM to accept them. Two fundamental classes are P and NP. A language L is in P (resp. NP) if there exists a deterministic (resp.
non-deterministic) TM accepting $L$ with computations that take a number of steps polynomial in the length of $w$ (polynomial-time computations). P is obviously contained in NP.

We now turn to the correspondence between Turing Machines and Bounded Tiling. The first step is to notice that, since we only consider finite time computations, we can assume that our TMs operate on a tape whose length is at most the size of the input plus the computation time. Second, without loss of generality we can restrict to computations such that the initial ID has the head facing the leftmost cell of the tape, and, when accepting, the final ID is

$$q_F, \#, \#, \ldots$$

A set of tiles can be associated with the program, and a row of tiles with each ID of a computation as follows. The first ID of the computation is associated with the row of tiles exhibited on Figure 3. The set of allowed tiles is the one reported below in Figure 4. For the $(|K|, |\Sigma|) = (5, 7)$ UTM mentioned above, the set of colours has size $|K| \times |\Sigma| + |K| + |\Sigma| + 1 = 48$. We notice how the set of tiles of Fig. 4 enforces any two adjacent rows representing IDs to be consistent. It is by now obvious that given an input $w$, there exists an accepting computation iff there exists a valid tiling associated with the boundary condition represented on Fig. 5.

Let $h_w$ and $\ell_w$ respectively denote the height and the length of the tiling for a given input size $|w|$. We assume that these two quantities grow polynomially with $|w|$. Consider now the problem of deciding if there exists a valid bounded tiling of size $h_w \times \ell_w$, where the boundaries are fixed as in Figure 5. Then it is easy to verify that a tiling exists if and only if there exists an $h_w$-step computation of the UTM accepting $w$. This implies that there is an efficient BT encoding for any NP problem. Therefore the ability to solve BT leads to an solution of any NP problem, i.e. BT is NP-hard.

Conversely, one can show that BT is in NP. Indeed, the notion of certificates for languages in NP (see Section 2.1), easily provides a deterministic Turing Machine verifying BT in polynomial time given a certificate. (An example for BT is a solution itself.) From this, a standard construction gives a non-deterministic TM that accepts the input iff a certificate (and therefore a solution) exists.

In conclusion, BT is NP-complete.

If $j = k - 1$ and $M = L$, place $q_j'$ on position $j$

If $j = k + 1$ and $M = R$, place $q_j'$ on position $j$

If $j = k$ and $M = 0$, place $q_j'$ on position $j$

If $j = k$ and $M = L$, place $q_j'$ on position $j$

If $j = k$ and $M = R$, place $q_j'$ on position $j$

Else, place $s_j$ on position $j$

Figure 4. The set of allowed tiles, to which we need to add the empty tile and the tiles with just the top or bottom color corresponding to a symbol from $\Sigma$ or $\Sigma \times K$.

Figure 3. The first row of tiles, corresponding to the initial ID.

Figure 5. The boundary conditions for the reduction. On the bottom, there is the initial ID, and on the top we enforce the accepting ID.

Appendix B: Undecidability

We briefly review the two notions of undecidability. A detailed explanation can be found in [4].

Definition 1. A problem is algorithmically undecidable if there is no algorithm running on a Turing machine that terminates and provides the correct answer for every instance.

We stress that a problem can only be undecidable if it has infinitely many instances. Indeed, if the problem has a finite number $\nu$ of instances, consider all the functions $f : \{1, \ldots, \nu\} \ni x \mapsto f(x) \in \{0, 1\}$. To each such function $f$, associate an algorithm where one prints YES if $f(x) = 0$, and NO else. Amongst the $2^\nu$ such functions, there is...
one that provides the correct answer for every instance: the problem is decidable.

**Definition 2.** A problem is axiomatically undecidable if given a set of axioms together with a set of rules to construct formal proofs, a statement can be neither proven nor disproven from the axioms.

One can prove there is a relation between these two notions [5]. If a decision problem is algorithmically undecidable, then for any consistent and recursive formal system in which the problem can be stated, there are infinitely many instances that can neither be proven nor disproven from the axioms. In this paper, we are mainly concerned with algorithmic undecidability.

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