Projected Entangled Pair States: Fundamental Analytical and Numerical Limitations

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Matrix product states and projected entangled pair states (PEPS) are powerful analytical and numerical tools to assess quantum many-body systems in one and higher dimensions, respectively. While matrix product states are comprehensively understood, in PEPS fundamental questions, relevant analytically as well as numerically, remain open, such as how to encode symmetries in full generality, or how to stabilize numerical methods using canonical forms. Here, we show that these key problems, as well as a number of related questions, are algorithmically undecidable, that is, they cannot be fully resolved in a systematic way. Our work thereby exposes fundamental limitations to a full and unbiased understanding of quantum many-body systems using PEPS.

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Matrix product states (MPS) have proven highly successful in the study of interacting of one-dimensional (1D) quantum systems. The explanation of the Density Matrix Renormalization Group method—the method of choice for the simulation of 1D systems—as a variational method over the manifold of MPS has triggered the development of a plethora of new methods, such as for the simulation of time evolution, excitations, or thermal states, as well as generalizations to higher dimensions using projected entangled pair states (PEPS) [1–4]. As their analytical understanding progressed, MPS were also exploited for analytical studies, and have in particular led to a full and rigorous classification of entangled phases under symmetries ("SPT phases") in 1D [5–7].

At first sight, this success is rooted in the fact that MPS provide a faithful approximation to low-energy states of physical systems by capturing their entanglement structure [8–10]. Nonetheless, a number of seemingly technical developments were central in turning this basic idea into the powerful numerical and analytical framework it is today; remarkably, those insights were later found to be intimately related to the fundamental structure of MPS. First, in order to render the variational optimization stable, the use of suitable *canonical forms* is needed, which, e.g., remove singularities in the normalization or redundant degrees of freedom [2,11]. Second, in simulating systems with symmetries, those symmetries are often explicitly encoded: This speeds up the method, allows us to reach significantly higher accuracies, ensures that the variational state is perfectly symmetric, and provides means to directly extract signatures of SPT order [2,12–16]. Crucially, the possibility to numerically utilize symmetries hinges on the fact that in MPS, any global symmetry of a wave function can be implemented locally, that is, at the level of the individual tensor which describes a single site [17–19].

Concurrently, it was understood that the local encoding of symmetries in MPS makes them an extraordinarily powerful analytical tool. Most importantly, the classification of all such encodings has provided us with a comprehensive classification of all phases in 1D under symmetries [5–7]. This success relies on two crucial points: First, the exhaustive knowledge of all ways in which any given symmetry can act in MPS, and second, the ability to interpolate between any two MPS in the same phase such

that along the whole interpolation, there is a smooth, gapped parent Hamiltonian.

Both numerical and analytical uses of symmetries hinge on a point of utmost importance: We must be absolutely certain that we consider all the possible ways in which symmetries of a 1D system can be encoded locally in the MPS. Otherwise, any classification would risk missing out on part of the possible phases, and correspondingly, numerical methods would be biased and possibly even unable to capture certain phases. Fortunately, a full characterization of all symmetry realizations in MPS is indeed known: It follows from the "fundamental theorem of MPS," which fully characterizes how two different MPS representing the same state—such as obtained by acting with a symmetry—are related, and which in turn is intimately connected with the aforementioned canonical forms relevant for numerical stability [2,17–19].

PEPS, the 2D analog of MPS, similarly form a faithful ansatz for low-energy states in 2D [20,21]. Numerical PEPS algorithms are progressing rapidly, even though canonical forms analogous to 1D are lacking [3,22,23]. Given the increased complexity in 2D, making use of symmetries is even more important. Generally, this is done using a straightforward generalization from 1D, where symmetries act on all entanglement degrees of freedom independently [12–14,24]. For a long time, this was the only symmetry realization considered, and thus, it came as a big surprise when Chen, Liu, and Wen devised a model where the symmetry, though local, acted in a correlated way on the entanglement degrees of freedom, and showed that this constituted a nontrivial SPT phase in 2D [25,26]. Subsequently, such correlated symmetry actions have been found to also underlie topologically ordered phases [27–29]. This contested how to encode symmetries in PEPS in the most general way—a question which is not only central to a comprehensive classification of phases, but yet again equally for the use of symmetries in numerical simulations, such as to guarantee an unbiased approach. Thus, an analogous "fundamental theorem of PEPS," which elucidates the most general way to realize symmetries in PEPS, is highly desirable.

In this Letter, we show that such a result cannot exist: It is impossible to fully characterize all the ways in which symmetries can be realized in PEPS—whatever list of possible realizations one has, it can never be complete. The reason is that, as we show, the question whether a PEPS has a certain symmetry is undecidable, that is, there is no algorithm which, given a PEPS tensor, can ever decide whether the family of states generated by that tensor will be symmetric. In particular, this rules out the possibility to have a list of possible symmetry realizations which can be systematically checked. This implies that we cannot just use PEPS for the classification of all possible phases, as we would risk losing certain symmetry realizations: For the very least, we would have to impose additional structure, such as to a physically motivated subclass of PEPS, but it could just as well be entirely impossible. Similarly, this implies that in numerical study, imposing symmetries locally through the tensor will always rule out certain symmetric states, even if we try to include as many symmetry realizations as possible. As a consequence, our no-go result implies the impossibility of a fundamental theorem of PEPS.

A key primitive in our argument is the problem of assessing if a PEPS is normalizable—that is, given a PEPS tensor, does it describe a state with nonzero norm? This problem in fact is already of interest on its own: A main reason for using canonical forms in numerical simulations is to avoid divergences in the normalization of the state. In PEPS simulations, such ill-conditioned behavior which could be tied to convergence of the method to non-normalizable states has indeed been observed [30,31]. As we show, this problem by itself is undecidable, that is, there is no algorithm which can ensure that a given PEPS tensor gives rise to properly normalizable states, thereby avoiding singularities and stabilizing numerical simulations. And finally, the undecidability of this key primitive has also another consequence, relating to the classification of phases using PEPS: One part of such a classification is the ability to connect two PEPS in the same phase along a smooth and gapped path [7]. However, we show that generally, the gap of such a parent Hamiltonian of a PEPS is undecidable as well. While this does not rule out suitable interpolations—they have to be constructed in a way which circumvents those cases—it exposes yet another limitation on the use of PEPS in a full classification of phases.

Let us start by reviewing the formalism of PEPS. A translational invariant PEPS (iPEPS) is characterized by a five-index tensor $A \equiv A^i_{\alpha\beta\gamma\delta}$ with physical index i and virtual or entanglement indices $\alpha, \ldots, \delta$. This tensor generates a family of states on systems of arbitrary size $N_h \times N_v$ (and thus asymptotically on the infinite plane) as follows: We arrange the tensor A in an $N_h \times N_v$ grid and contract (that is, identify and sum over) adjacent indices, indicated by connected lines in Fig. 1(b), and terminate the virtual indices at the boundary with some boundary condition. The resulting object now only depends on the physical indices $\boldsymbol{i} = (i_{1,1}, \ldots, i_{N_h,N_v})$, and we denote it by $\mathcal{C}_A(\boldsymbol{i})$. It defines a quantum state—the PEPS—by virtue of $|\Psi_{N_h,N_v}\rangle = \sum_{\boldsymbol{i}} \mathcal{C}_A(\boldsymbol{i})|\boldsymbol{i}\rangle$. In principle, $\mathcal{C}$ still depends on the boundary conditions. However, for a well-defined

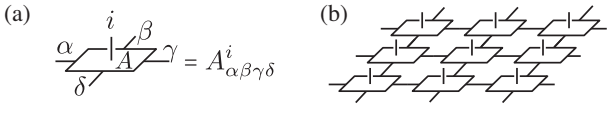

FIG. 1. PEPS construction: A five-index tensor (a) is used to describe a wave function on an infinite lattice by contracting the virtual indices $\alpha, \beta, \ldots$, as indicated.

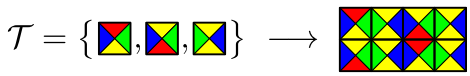

FIG. 2. The tiling problem: Can a set of tiles tile the plane?

thermodynamic limit both in numerical simulations and in a rigorous mathematical sense, we must demand that properties in the bulk become independent of the chosen boundary condition, except for possibly selecting a symmetry broken sector.

A key tool in our work will be the tiling problem [32], Fig. 2. It is specified by a set of square tiles $\mathcal{T} = \{t_i\}_{i=1}^{T}$, which are colored in a way where each edge $e = l, u, r, d$ is assigned a color c_e, $t \equiv (c_l, c_u, c_r, c_d)$. The tiling problem now asks to cover a given region with those tiles (without rotating), such that the colors of two adjacent tiles agree on shared edges. Tiling problems can be mapped to a tensor network in a natural way: To this end, choose the dimension of the physical index equal to the number of allowed tiles $|\mathcal{T}|$, and define a tensor

$$A^{t}_{\alpha_l\alpha_u\alpha_r\alpha_d} = 1 \quad \text{if } t = (\alpha_l, \alpha_u, \alpha_r, \alpha_d), \tag{1}$$

and zero otherwise.

What does this construction imply for the PEPS $|\Psi_{\text{tile}}\rangle$ constructed from A on a patch $N_h \times N_v$? Consider two adjacent tensors $A^{t}_{\alpha_l\alpha_u\alpha_r\alpha_d}$ and $A^{t'}_{\beta_l\beta_u\beta_r\beta_d}$ with tiles $t = (c_l, c_u, c_d, c_r)$ and $t' = (c'_l, c'_u, c'_d, c'_r)$, where the former is to the left of the latter. Contracting the tensors means setting $\alpha_r = \beta_l$ and summing. But since $\alpha_r = c_r$ and $\beta_l = c'_l$, this implies $c_r = c'_l$, summed over all possible values. Thus, the adjacent tile colors of the tensors must match, and can take any allowed value—by construction, the tensors automatically enforce the tiling rules. It is now easy to see that this pattern persists as one continues to contract indices. Specifically, if the coloring $\boldsymbol{t} = (t_{1,1}, \ldots, t_{N_h,N_v})$ is inconsistent, then $\mathcal{C}_A(\boldsymbol{t}) = 0$, and otherwise, $\mathcal{C}_A(\boldsymbol{t}) = \langle \boldsymbol{\alpha} | b \rangle$, where $\boldsymbol{\alpha}$ is the boundary coloring of $\boldsymbol{t}$, and $|b\rangle$ the boundary condition imposed.

A second way to map tiling problems to PEPS is to choose $\tilde{A}^{i}_{\alpha_l\alpha_u\alpha_r\alpha_d} = 1$ if $i = 0$ and $(\alpha_l, \alpha_u, \alpha_r, \alpha_d) \in \mathcal{T}$, and zero otherwise: This construction yields a PEPS description $|\tilde{\Psi}_{\text{tile}}\rangle$ of a product state $|0\rangle^{\otimes N}$ (or, alternatively, a tensor network without physical indices), where the normalization equals the number of all consistent tilings; again, if there is no consistent tiling, the norm of this PEPS is zero. Clearly, $|0\rangle$ can be replaced with any other state.

A key result on tiling problems relates to the following: Given a set of tiles, is it possible to use them to tile the infinite plane—that is, to tile regions of arbitrary size $N_h \times N_v$, if we don't impose boundary conditions—or is there a size above which no allowed tiling exists? It has been shown that this problem is (algorithmically) undecidable, that is, there is no algorithm which runs in finite time (no matter how slow) which will solve this question for an arbitrary set of allowed tiles [32,33]. Let us now apply this result in the light of our tiling to PEPS mapping: Since $\mathcal{C}_A(\boldsymbol{t})$ can be nonzero only for allowed tilings, the impossibility to tile the plane implies that there is a size $N_h \times N_v$ above which the PEPS defined by the tensor A, Eq. (1), is identically zero (that is, non-normalizable), *regardless* of the choice of boundary conditions. On the other hand, if a valid tiling exists, the state will be nonzero for a suitable boundary condition, such as the uniform superposition of all colors. We thus find that the following problem is undecidable:

Undecidable problem 1: PEPS zero testing.—Given a tensor A, is there a choice of boundary conditions such that the PEPS constructed from A is nonzero for all system sizes?

Note that the boundary conditions are allowed to depend on the system size. Importantly, the nonexistence of such boundary conditions in particular implies that the PEPS described by A is ill defined in the thermodynamic limit. Using the second construction above, this result even holds for PEPS without a physical index (or nontrivial PEPS representations of product states).

As explained, this problem is of considerable interest by itself to prevent PEPS algorithms to run into singular points; our result shows that there is no algorithm which will circumvent this problem in the general case. However, it will, moreover, serve us as an elementary building block to assess the difficulty of central problems in the field of PEPS, most importantly the realization of symmetries and the existence of a fundamental theorem.

We start by considering the problem of how to implement symmetries in PEPS in full generality. As outlined above, a comprehensive understanding is essential both for a complete classification of phases and for a fair and unbiased implementation of symmetries in numerical simulations. First off, we need to clarify what it means for an iPEPS to be symmetric. To start with, let us consider an on-site symmetry $\mathcal{S}_g = U_g^{\otimes N}$, $g \in G$, which is unbroken. A PEPS tensor provides a "good" description of an infinite system if it yields a well-defined limit as we increase the system size, independent of the boundary condition we choose. This is both true in numerical simulations, where we require well-defined corner transfer matrix (CTM) or infinite MPS (iMPS) fixed points [3,22,23], as well as the correct formal definition in mathematical physics. Specifically, for a symmetric PEPS, this means that the reduced density matrix ρ_R of any region R, in the limit where the boundaries are far away, is unique and thus invariant under the symmetry, $\mathcal{S}_g \rho_R \mathcal{S}_g^{\dagger} = \rho_R$. This characterization generalizes immediately to other symmetries, such as reflection, time-reversal, or translation (in the last case, ρ_R has to be invariant under translation of R); and can be generalized to broken symmetries, where ρ_R can depend on the boundary condition only to the extent that the boundary selects a symmetry broken sector.

Now consider an arbitrary PEPS $|\Theta_{\mathrm{sym}}\rangle$ with tensors $B^i_{\alpha_l\alpha_u\alpha_r\alpha_d}$ which is invariant under the symmetry $\mathcal{S}_g$ in the sense above. In addition, take a product state which is *not* invariant under $\mathcal{S}_g$ for some g (such a state always exists, possibly not translation invariant if point or space group symmetries are included), and construct a PEPS description $|\tilde{\Psi}_{\mathrm{tile}}\rangle$ (with tensors $\tilde{A}^i$) of this product state, following the mapping from the tiling problem described above, for which the question $|\tilde{\Psi}_{\mathrm{tile}}\rangle \stackrel{?}{=} 0$ is undecidable. We can now combine these two PEPS into a single PEPS

$$|\Phi_{\mathrm{sym?}}\rangle = |\tilde{\Psi}_{\mathrm{tile}}\rangle + |\Theta_{\mathrm{sym}}\rangle;$$

its PEPS tensor C is obtained as the direct sum of $\tilde{A}^i$ and B^i (that is, the virtual space is the direct sum of the two virtual spaces, $C^i = \tilde{A}^i$ exactly if all virtual indices are in the $\tilde{A}$ part of the direct sum, $C^i = B^i$ exactly if all are in the B part, and $C^i = 0$ otherwise). Let us now consider the two cases which are undecidable to distinguish: First, there is a valid tiling, and thus $|\tilde{\Psi}_{\mathrm{tile}}\rangle \neq 0$ for some suitable boundary condition for any system size—in that case, the reduced density matrix ρ_R of $|\Phi_{\mathrm{sym?}}\rangle$ will depend on the boundary conditions, and in particular, there exist boundary conditions supported in the $\tilde{A}^i$ sector for which ρ_R will not be symmetric. Second, there is no valid tiling of the plane, and thus $|\tilde{\Psi}_{\mathrm{tile}}\rangle \equiv 0$ for large enough systems—then, for any boundary condition, ρ_R will only have contributions from $|\Theta_{\mathrm{sym}}\rangle$, and thus be symmetric. We therefore find that the following problem is undecidable:

Undecidable problem 2: Symmetries in PEPS.—Given a tensor C and a symmetry $\mathcal{S}_g$, $g \in G$, is the translational invariant PEPS constructed from C invariant under $\mathcal{S}_g$ in the thermodynamic limit?

Note that this result holds for any symmetry representation, and thus, e.g., already for spin-$\frac{1}{2}$ systems.

This undecidability statement has profound implications for the classification of symmetry encodings in PEPS. In particular, it tells us that there cannot be a comprehensive list of all possible ways to encode symmetries in PEPS which can be checked by any algorithm (regardless how inefficient), since otherwise, there would be an algorithm deciding the presence or absence of symmetries in a given PEPS. Therefore, any classification of symmetries in PEPS, and thus any classification of phases under symmetries, must rely on some assumptions about the way in which the symmetry is encoded, or in some other way restrict to a subclass of PEPS with additional structure.

A direct consequence is the impossibility to have a fundamental theorem of PEPS which relates two different PEPS representations of the same state.

Undecidable problem 3: Fundamental Theorem for PEPS.—Given tensors A^i and B^i, decide if they describe the same PEPS for any system size.

Here, "describe the same PEPS" is meant in the same way as for symmetries, namely, that the reduced density matrices of the two states become indistinguishable as the boundaries are taken to infinity. The proof is immediate since by choosing $B^i = \sum (U_g)_{ij} A^j$, we see that the case of deciding symmetries (undecidable problem 2) is a special case. Importantly, this implies that there is no algorithm to bring PEPS into a canonical form from which we can algorithmically decide whether they describe the same state, let alone find a local gauge transformation relating A^i and B^i.

Finally, we can employ our construction to show that verifying whether a PEPS parent Hamiltonian is gapped is an undecidable problem. As discussed in the introduction, PEPS come naturally with parent Hamiltonians [34,35], and in 1D, the fact that those Hamiltonians are uniformly gapped is a crucial ingredient in the classification of phases, as it allows us to connect two states in the same phase through a gapped path of MPS [7]. However, in 2D, the corresponding problem is undecidable:

Undecidable problem 4: Gap of parent Hamiltonians.—For the parent Hamiltonian H_N of a PEPS with open boundaries on an $N \times N$ patch, it is undecidable to distinguish between the following two cases: (i) H is gapped—specifically, there exists an N_0 such that for all $N \geq N_0$, H has a spectral gap $\Delta \geq 1$ above the ground state; (ii) H is gapless—specifically, the spectrum of H converges to $[0; \infty)$.

The proof proceeds by constructing a PEPS which is a superposition of a PEPS with a gapped parent Hamiltonian and a PEPS with a gapless parent Hamiltonian, coupled to a tiling PEPS without physical indices. This way, whenever there does not exist a tiling, we obtain the first state and thus a gapped Hamiltonian, while otherwise, the other state appears and gives rise to a gapless parent Hamiltonian (see Supplemental Material for details [36]). Note that this strengthens the existing undecidability result for spectral gaps [42], as it shows it even holds when restricting to PEPS parent Hamiltonians.

Finally, the mapping between tilings and PEPS, applied to finite systems with fixed boundary conditions, allows for straightforward proofs of the computational hardness of certain problems, such as finding ground states and zero testing, presented in the Supplemental Material [36].

In conclusion, we have studied the difficulty of some central problems in the field of PEPS, relevant both for their use as an analytical framework and as a powerful numerical tool. By establishing a mapping between tiling problems and PEPS, combined with the existence of undecidable tiling problems, we were able to establish undecidability of a range of these problems. Specifically, we could show that the problem of deciding whether a PEPS is invariant under a given symmetry, as well as the problem of deciding whether two PEPS tensors represent the same state, are undecidable. In particular, this implies the impossibility to succinctly enumerate all ways in which a symmetry can be encoded locally in the PEPS tensor, and thus exposes

fundamental limits to the possibility of performing unbiased analytical and numerical analysis of PEPS with symmetries. As a technical result with implications on its own right, we could, moreover, show that the problem of deciding whether a PEPS tensor actually describes a physical (that is, nonzero and thus normalizable) state is undecidable as well; and finally, we have shown how this implies undecidability of a spectral gap in the case of PEPS parent Hamiltonians. Let us note that these limitations, while severe, can potentially be overcome by restricting to a physically relevant subclass of PEPS, such as the states which appear in approximation proofs or numerical simulations, and which likely carry additional structure which could potentially allow to overcome those restrictions.

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