Internal structure of gauge-invariant Projected Entangled Pair States

David Blanik,[1] José Garre-Rubio,[2,3] András Molnár,[2] and Erez Zohar[4]

[1]*University of Vienna, Faculty of Physics, Boltzmanngasse 5, 1090 Vienna, Austria*
[2]*University of Vienna, Faculty of Mathematics, Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria*
[3]*Instituto de Física Teórica, UAM/CSIC, Universidad Autónoma de Madrid, Madrid, Spain*
[4]*Racah Institute of Physics, The Hebrew University of Jerusalem, Givat Ram, Jerusalem 91904, Israel*
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Projected entangled pair states (PEPS) are very useful in the description of strongly correlated systems, partly because they allow encoding symmetries, either global or local (gauge), naturally. In recent years, PEPS with local symmetries have increasingly been used in the study of non-perturbative regimes of lattice gauge theories, most prominently as a way to construct variational ansatz states depending only on a small number of parameters and yet capturing the relevant physical properties. For the case of one-dimensional PEPS (Matrix Product States — MPS) a bidirectional connection was established between the internal structure of the tensor network, i.e. the mathematical properties of the constituent tensors, and the symmetry. In higher dimensions this has only been done for global symmetries, where in the local (gauge) case it is known only how to construct gauge-invariant states, but not what the symmetry implies on the internal structure of the PEPS. In the present work we complete this missing piece and study the internal structure of projected entangled pair states with a gauge symmetry. The PEPS we consider consist of matter and gauge field tensors placed on the vertices and edges, respectively, of arbitrary graphs.

I. INTRODUCTION

The role of gauge theories in modern physics cannot be underestimated. Having local symmetries at their core, they describe matter minimally coupled to gauge fields acting as interaction mediators. This quantum field theoretic description [1] is central to the Standard Model of particle physics [2], as well as several effective models of condensed matter [3].

However, quantum gauge field theories, particularly non-abelian ones, are notoriously difficult to study in their non-perturbative regimes. One successful approach involves the latticization of the theory, as proposed by Wilson [4], which, when combined with Monte Carlo techniques [5], allows the computation of many important static quantities; for example, the hadronic spectrum of quantum chromodynamics (see, e.g., the review [6]). This approach, however, faces significant challenges when dealing with two specific, physically important scenarios. First, it does not allow the direct description of real-time evolution, since Monte Carlo computations are performed within a Euclidean, Wick-rotated spacetime. Second, at finite fermion density, the sign problem [7] may occur, blocking the way for Monte-Carlo studies of exotic phases, including many physically relevant regions of the QCD phase diagram [8].

One relatively recent way of tackling these issues, and in particular overcoming the sign problem, which is specific to path-integral Monte Carlo computations, is the use of tensor network states. Tensor network states (TNS) [9–12] are constructed from local tensors placed at particle sites (usually vertices or edges of the lattice) mimicking the interactions between them. The size of these local tensors determines how well the TNS approximates a given state. Crucially, TNS constructed from local tensors of only moderate size are already well suited to approximate states satisfying an entanglement area law, expected to hold for physically relevant states (e.g., ground states of local gapped Hamiltonians [13–16]), allowing for efficient numerical computations. In the context of lattice gauge theories, two (and higher) dimensional tensor networks, and in particular projected entangled pair states (PEPS) [12, 17], have been applied to the Hamiltonian formulation, introduced by Kogut and Susskind [18]. In one space dimension, the family of TNS known as matrix product states (MPS) have been successfully applied to several lattice gauge theory models (see, e.g., the earlier works [19–25] as well as the review papers [26–28]). In higher dimensions, either tree tensor networks or infinite PEPS are used [29–37] — both are very powerful numerical techniques, though not necessarily tailored to the symmetries present in such models. A parallel, non-Hamiltonian approach is that of the Tensor Renormalization Group (TRG) method, as described in detail in the review [38].

Other approaches are based on the gauging of globally symmetric PEPS [39, 40], where one lifts the global symmetry to a local one, creating ansatz states useful for lattice gauge theory computations. In particular, [40] suggested how this can be done in a way analogous to minimal coupling of free, globally invariant matter Hamiltonians or Lagrangians [1], where the lift is achieved by the introduction of gauge fields. It was shown that when the gauged state is a Gaussian fermionic PEPS [41], giving rise to states known as gauged Gaussian PEPS [42, 43], one can use variational Monte Carlo techniques for an efficient ground state search [44–47]. Therefore such gauged PEPS are useful in physical contexts and could be utilized in the study of the non-perturbative regime of lattice gauge theories. While the above works do well in providing methods to construct PEPS with gauge symmetries, one would like to understand the reverse direc-

tion as well — given a locally symmetric PEPS, how is the symmetry encoded in its local constituents? The way global properties of TNS, e.g., symmetries, are encoded in the local tensors is of high relevance to the study of such states (e.g., leading to the classification of 1D gapped phases [48, 49]).

This question has previously been addressed for a single space dimension, that is, for MPS [50], and in the present work we aim at extending their results to higher dimensions, arbitrary lattices, geometries or graphs. For several families of TNS, the local encoding of the symmetry can be extracted using a set of results known as Fundamental Theorems [51], however, fundamental obstructions [52] prevent a fully general analysis. Consequently, in this work we shall only consider PEPS with matter and gauge fields described by local tensors which become injective after blocking, a strong invertibility condition [11, 51]. This family is important because an injective PEPS with only matter degrees of freedom is the unique ground state of an associated local, gapped Hamiltonian [53], known as the parent Hamiltonian.

The structure of the paper is as follows. We begin in Section II by introducing the necessary background on tensor network states and their graphical notation. Then in Section III we analyze the very simplest non-trivial example of a PEPS on the square lattice. This section only serves to illustrate the main ideas of our method in a simple setting. In Section IV we state and prove our main technical lemma, a slightly stronger variation of the Fundamental Theorem of injective MPS, established in [51]. Finally, in Section V we state and prove our results in the most general setting we have been able to analyze.

II. BASICS ON TENSOR NETWORKS AND GRAPHICAL NOTATION

Tensor network states are constructed via the concatenation of local tensors, often placed on the vertices and/or edges of a regular lattice. We explain the key concepts of this construction on the very important example of matrix product states (MPS) in the setting of spin chains [11]. A (translation invariant) MPS is defined by a 3-index tensor B where one index corresponds to the local Hilbert space $\mathbb{C}^d$ and the other two are associated with the so-called virtual or auxiliary level with bond dimension D. The tensor B can be seen as a collection of d matrices, each of size $D \times D$: $\{B^i, i = 1, \ldots, d\}$. Then the MPS on n sites constructed with the tensor B is given by:

$$|\Psi(B)\rangle_n = \sum_{i_1, \ldots, i_n} \mathrm{Tr}\{B^{i_1} \cdots B^{i_n}\} |i_1, \ldots, i_n\rangle. \quad (1)$$

From a slightly more abstract point of view, which we shall adopt below, one considers the MPS tensor B to be an element of the tensor product of the physical and virtual Hilbert spaces, which will also be defined below. The

importance of this class of TNS stems from the ability of MPS to efficiently approximate ground states of local, gapped Hamiltonians, which follows from the fact that both satisfy an entanglement entropy area law [13, 14].

In order to generalize this construction to higher dimensions we will first introduce the graphical notation of tensors. A tensor is depicted by a shape, usually a circle, with as many legs as indices, where the indices should be thought of as corresponding to a choice of basis on the Hilbert space associated with the leg. There are two basic operations between the indices of (different) tensors. The first one is the contraction of two indices where the labels are identified and summed over. An example is matrix multiplication: $(fg)_{ij} = \sum_{kl} \delta_{kl} f_{ik} g_{lj}$. The graphical representation of the contraction is to glue or concatenate the legs of the involved indices together. This operation corresponds to the natural pairing between a Hilbert space and its dual and can in some cases be viewed as composition of functions, c.f. Figure 1(b). The second operation is blocking: here multiple indices, or Hilbert spaces, are considered as one, so that their total dimension is the product of the individual ones. An example is the tensor product of matrices or operators, $f \otimes g$, c.f. Figure 1(a). The higher-dimensional generalization of MPS are called projected entangled pair states (PEPS). For the two-dimensional square lattice the tensors of a PEPS are rank 5 (5 indices) and they are placed on the vertices, c.f. Figure 1(c, d). Notice the simplicity of the graphical notation; the corresponding algebraic expression is too complicated to be written down here.

Figure 1. In graphical notation the tensor product (a) of operators is depicted by simply drawing the factors next to each other. Composition (b), or more generally contraction, is depicted as concatenation of diagrams, where the ordering is determined by the orientation of the legs. We depict a rank 5 tensor (c) and how it can be used to construct a PEPS on a square lattice (d), given the virtual Hilbert spaces are chosen appropriately. Similarly, a rank 3 tensor (e) can be used to construct a translation invariant MPS (f) with periodic boundary conditions.

Definition II.1 (MPS). Formally, in TN diagrams a Hilbert space is assigned to each edge (or leg) and tensors, being nodes where multiple edges meet, are simply elements in the tensor product of the Hilbert spaces as-

sociated with its incident legs, e.g.,

$$B \equiv \ \overset{\mathcal{H}}{\underset{B}{\ominus}}\ \equiv\ \mathcal{V}_{\mathrm{o}}\ \overset{\mathcal{H}}{\underset{B}{\ominus}}\ \mathcal{V}_{\mathrm{t}}\ \in \mathcal{V}_{\mathrm{o}} \otimes \mathcal{H} \otimes \mathcal{V}_{\mathrm{t}}^{*}, \quad (2)$$

where the dual of a Hilbert space appears in the tensor product, if the edge it is associated with terminates at the tensor.

Hilbert spaces denoted as $\mathcal{H}$ we shall refer to as *physical*, while Hilbert spaces denoted as $\mathcal{V}$ we shall refer to as *virtual*. Equation (2) depicts the prototypical example of an MPS tensor, where we denote the virtual Hilbert spaces $\mathcal{V}_{\mathrm{o}}$ and $\mathcal{V}_{\mathrm{t}}$, because they are associated with edges that have the MPS tensor as their origin and terminus, respectively.

Definition II.2 (Injectivity). An MPS tensor B, defined according to Equation (2), is called

(i) *injective*, if it is injective as a map[1]

$$\overset{}{\underset{B}{\ominus}} : \mathcal{V}_{\mathrm{o}}^{*} \otimes \mathcal{V}_{\mathrm{t}} \longrightarrow \mathcal{H}. \quad (3)$$

(ii) *left injective*, if it is injective as a map

$$\overset{}{\underset{B}{\ominus}} : \mathcal{V}_{\mathrm{t}} \longrightarrow \mathcal{V}_{\mathrm{o}} \otimes \mathcal{H}. \quad (4)$$

(iii) *right injective*, if it is injective as a map

$$\overset{}{\underset{B}{\ominus}} : \mathcal{V}_{\mathrm{o}}^{*} \longrightarrow \mathcal{H} \otimes \mathcal{V}_{\mathrm{t}}^{*}. \quad (5)$$

(iv) *unital*, if $\mathcal{V}^{\mathrm{o}} = \mathcal{V}^{\mathrm{t}} =: \mathcal{V}$ and there exists $x \in \mathcal{H}^{*}$ such that

$$\overset{\bullet\,x}{\underset{B}{\ominus}} = \mathrm{id}_{\mathcal{V}}. \quad (6)$$

If a tensor satisfies (ii) and (iii), we call it *LRI*. In components, unitality just means $\sum_{i} x_{i} B^{i} = \mathbb{1}$.

Remark. Injective $\Rightarrow$ unital $\Rightarrow$ LRI.

Part (i) of the previous definition is standard [11] and Lemma II.1 justifies the introduction of notions (ii) and (iii). Part (iv) is convenient to give examples. Clearly,

injectivity of the tensor B is equivalent to the existence of a tensor B^{-1}, often called the *inverse* of B, satisfying

$$\overset{B^{-1}}{\underset{B}{\ominus}} \ = \ \bigg]\bigg[\ \equiv \mathrm{id}_{\mathcal{V}_{\mathrm{o}}^{*}} \otimes \mathrm{id}_{\mathcal{V}_{\mathrm{t}}}, \quad (7)$$

where in the last equality we view the TN diagram as a linear map going from bottom to top.

Lemma II.1. Let T be an injective[2] tensor. For any MPS tensor B the following equivalences hold:

$$\overset{B}{\underset{T}{\ominus}} \quad \text{injective} \quad \Leftrightarrow \quad B \text{ is left injective}, \quad (8)$$

$$\overset{B}{\underset{T}{\ominus}} \quad \text{injective} \quad \Leftrightarrow \quad B \text{ is right injective}. \quad (9)$$

Proof. To prove (8, $\Rightarrow$), assume B is not left injective, which implies the existence of $x \in \mathcal{V}_{\mathrm{t}}$ such that

$$\overset{}{\underset{B}{\ominus}}\!\!\bullet x\ = 0, \quad (10)$$

which is of course in contradiction to the injectivity of the composite tensor. The reverse implication (8, $\Leftarrow$) follows immediately after contracting the composite tensor with the inverse of T. One proves (9) in a completely analogous manner. $\square$

Hence, blocking with B preserves injectivity precisely if it is left and/or right injective.

III. EXAMPLE: NORMAL PEPS ON SQUARE LATTICE

As a simple first example, to illustrate the ideas appearing in the proof of the general statement in Section V, we consider a gauge-invariant PEPS on a square lattice with periodic boundary conditions, i.e. defined on the underlying geometry of a torus.

Such a state is constructed by placing rank 5 tensors A_{v}, which we think of as describing the matter degrees of freedom, at each vertex v and rank 3 tensors B_{e}, which we think of as describing the gauge degrees of freedom, at each edge e of the lattice. The physical local Hilbert spaces, always associated with the first leg of each tensor, are denoted $\mathcal{H}_{v}$ and $\mathcal{H}_{e}$, respectively.

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[1] When interpreting TN drawings as linear maps, we shall usually view them as going from bottom to top.

[2] A PEPS tensor is called *injective* if it is injective as a map from virtual to physical Hilbert spaces, c.f. Definition V.4.
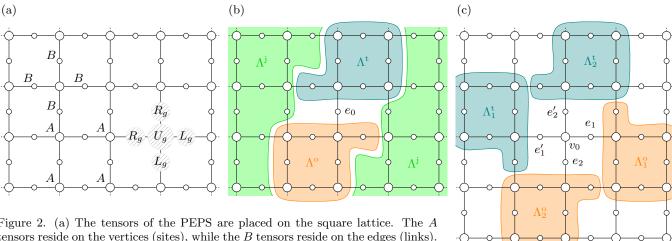
Figure 2. (a) The tensors of the PEPS are placed on the square lattice. The A tensors reside on the vertices (sites), while the B tensors reside on the edges (links). The gauge symmetry acts, indicated by the shaded regions, on a vertex and on its surrounding edges. (b) Isolating a single gauge tensor B at edge e_0 from the rest of the tensor network is achieved by selecting adjacent regions Λ^{o} and Λ^{t}, as indicated in the figure, in such a way that blocking the tensors contained within results in injective tensors. The region Λ^{j} contains the remainder of the lattice and can either be connected or disconnected. It is used only for bookkeeping purposes. The superscripts are meant to reference *origin*, *terminus* and *junk*, respectively, and we use the colors orange, teal and jade as a visual aid. When we don't explicitly indicate the orientation of the edges in drawings, they are usually implied to be oriented left to right and bottom to top. (c) To separate a single matter tensor A at vertex v_0 together with its surrounding gauge tensors, from the remaining tensor network we can employ the same regions we used above when isolating the edge tensors incident to v_0, since blocking the tensors contained within $\Lambda_1^{\mathrm{t}} \cup \Lambda_2^{\mathrm{t}} \cup \Lambda_1^{\mathrm{o}} \cup \Lambda_2^{\mathrm{o}}$, results in an injective tensor.

Contracting the remaining legs, corresponding to virtual degrees of freedom, according to the lattice geometry depicted in Figure 2(a), results in the state:

$$|\Psi(A,B)\rangle \in \bigotimes_v \mathcal{H}_v \otimes \bigotimes_e \mathcal{H}_e. \qquad (11)$$

Let G be a finite, or compact Lie group and consider representations[3] $U_v : G \to \mathrm{GL}(\mathcal{H}_v)$ and $L_e, R_e : G \to \mathrm{GL}(\mathcal{H}_e)$, for all vertices (sites) v and edges (links) e, where we require L and R to be commuting, i.e. $[R_e(h), L_e(g)] = 0$ for all edges e and $g, h \in G$. Saying the state $|\Psi(A,B)\rangle$ has a gauge symmetry simply means that (disregarding the case of static charges) it satisfies

$$\widehat{U}_v(g) |\Psi(A,B)\rangle = |\Psi(A,B)\rangle \qquad (12)$$

for all vertices v, with

$$\widehat{U}_v := R_{v_\mathrm{l}} \otimes R_{v_\mathrm{t}} \otimes U_v \otimes L_{v_\mathrm{r}} \otimes L_{v_\mathrm{b}}, \qquad (13)$$

where the subscripts denote the edges to the left, top, right and below of the vertex v, c.f. Figure 2 (a).

To simplify notation, we shall assume that all vertex tensors and edge tensors are equal, to be precise $A_v \equiv A$ and $B_e \equiv B$ for all v and e. This restriction is by no means necessary, but there is simply no insight to be

gained from considering the general case here. Graphically, we can depict property (12) for a single vertex as

$$
\begin{array}{c}
\includegraphics
\end{array}
\;=\;
\begin{array}{c}
\includegraphics
\end{array}, \qquad (14)
$$

where we use dotted lines to indicate that the equality involves the whole tensor network and not just the indicated tensors. We want to understand how the gauge symmetry of the PEPS is realized at the virtual level of the constituent tensors A and B, similar to what has already been established for MPS [50]. Given the well known fundamental obstructions [52], we do not expect to be able to solve this problem in full generality, but some extra assumptions on the tensors are needed to make progress. For this example we shall impose the following (unnecessarily strong) conditions:

(i) The vertex tensors become injective after blocking rectangular (say 2×2) regions, i.e. A is normal.

(ii) The edge tensor B is unital, c.f. Definition II.2(iv).

These conditions imply in particular that blocked tensors of the shape

$$
\begin{array}{c}
\includegraphics
\end{array} \qquad (15)
$$

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are injective. When we prove the general statement we will see that we can weaken these conditions substantially. Continuing now with the above conditions on the PEPS tensors it is straightforward to derive their local transformation properties under the gauge symmetry, by focusing first on the behavior of a single edge tensor. Fix an edge e_0 and consider regions Λ^{o}, Λ^{t} and Λ^{j}, as indicated in Figure 2 (b), and let $\mathbb{T}^{\mathrm{o}}$, $\mathbb{T}^{\mathrm{t}}$ and $\mathbb{T}^{\mathrm{j}}$, respectively, denote the tensors one gets after blocking the tensors inside these regions. Clearly the PEPS can now be written as an MPS

$$|\Psi(A,B)\rangle = \qquad = \qquad ,$$

where we do not draw the (many) physical legs of $\mathbb{T}^{\mathrm{j}}$. Notice that the blocked tensors $\mathbb{T}^{\mathrm{o}}$ and $\mathbb{T}^{\mathrm{t}}$ are of the form (15), hence injective, and that the gauge transformations involving e_0 act either on $\mathbb{T}^{\mathrm{o}}$ or $\mathbb{T}^{\mathrm{t}}$ but never on both and never on $\mathbb{T}^{\mathrm{j}}$, so with slight abuse of notation we can write for all $g \in G$
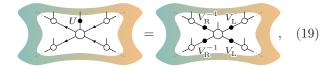
$$ \qquad = \qquad , \qquad (16) $$

where $\widetilde{U}(g) \otimes L(g) := \widehat{U}(g)$ and

$$ \qquad = \qquad , \qquad (17) $$

where $R(g) \otimes \widetilde{U}(g) := \widehat{U}(g)$. This means that the conditions of Lemma IV.1, to be stated and proved in the next section, are satisfied and we conclude the existence of unique, invertible matrices $V_{\mathrm{L}}(g)$ and $V_{\mathrm{R}}(g)$ such that

$$ \qquad = \qquad , \qquad \qquad = \qquad , \qquad (18) $$

for all $g \in G$. Furthermore, from the uniqueness we conclude that V_{L} and V_{R} constitute representations of G. Having established how the tensor B transforms under L and R, only leaves the transformation property of the tensor A, which is remarkably simple to derive now.

We shall again focus on a fixed vertex v_0. Notice that blocking the tensors contained in the regions Λ_1^{o}, Λ_2^{o}, Λ_1^{t} and Λ_2^{t}, as indicated in Figure 2 (c), yields four injective tensors, which we can invert to decouple the vertex tensor

A at v_0 and its surrounding B tensors from the rest of the lattice. Knowing how the tensors B transform under the symmetry operations we can write Equation (14) as

$$ \qquad = \qquad , \qquad (19) $$

where we have suppressed the explicit g dependence. Now we invert the surrounding injective region as well as the surrounding edge tensors and, after discarding the rest of the lattice, are left with

$$ \qquad = \qquad , \qquad (20) $$

for all $g \in G$. Equations (18) and (20) can be recognised as the symmetry conditions of gauge-invariant PEPS, c.f. [40]. There, it was shown that these conditions guarantee a construction of a gauge-invariant PEPS; here we prove the opposite direction.

IV. MAIN TECHNICAL LEMMA

In this section we prove a slightly stronger variation of the Fundamental Theorem of injective MPS [51]. We do so by generalizing the assumptions of the lemma to better apply to our specific situation. This lemma will be used to prove our general statement in section V.

Lemma IV.1 (Fundamental Lemma). Let A_{L} and A_{R} be injective MPS tensors and X an arbitrary non-zero tensor, which may even include additional not contracted (usually physical) legs. If B is a right injective MPS tensor and the symmetry property

$$ \qquad = \qquad \qquad (21) $$

holds, where L and U_{L} are invertible operators on the physical Hilbert spaces, then there exists a unique invertible matrix V_{L} such that

$$ \qquad = \qquad . \qquad (22) $$

Analogously, if B is a left injective MPS tensor and the symmetry property

$$ \qquad = \qquad \qquad (23) $$

holds, where R and U_R are invertible operators on the physical Hilbert spaces, then there exists a unique invertible matrix V_R such that

$$\begin{array}{cc} \underset{B}{\overset{R}{\bigcirc}} & = \underset{B}{\overset{V_R}{\bigcirc}} \end{array}. \tag{24}$$

Proof. We prove the statement for L and V_L. The proof for R and V_R is completely analogous. From Equation (21) and the fact that A_R is injective we conclude

$$ \tag{25} $$

where the unlabeled tensor can be arbitrary. Since we required B to be left injective, the inverse of $\overset{\bigcirc\ \bigcirc}{B\ A_R}$ is of the form $\overset{C\ A_R^{-1}}{\bigcirc-\bigcirc}$, and Equation (25) implies

$$ \tag{26} $$

Inserting Equation (26) back into (21) gives

$$ \tag{27} $$

and after inverting the injective tensors A_L and A_R we are left with (recall $X \neq 0$)

$$\begin{array}{cc} V_L \underset{B}{\overset{L}{\bigcirc}} & = \underset{B}{\bigcirc} \end{array}. \tag{28}$$

Notice that by the right injectivity of B, the matrix V_L satisfying Equation (28) has to be unique. What remains is to show that V_L is invertible. By the same reasoning that led to Equation (28), but inverting U_L instead of L in Equation (21), we get

$$\begin{array}{cc} V' \underset{B}{\overset{L^{-1}}{\bigcirc}} & = \underset{B}{\bigcirc} \end{array}, \tag{29}$$

for some matrix V'. Combining Equations (28) and (29) with the right-injectivity of B yields

$$\underset{V_L\ \ V'}{\bullet\bullet} = \underline{\quad\quad} = \underset{V'\ \ V_L}{\bullet\bullet}, \tag{30}$$

i.e. V' is the inverse of V_L. $\qquad\square$

V. GENERAL STATEMENT

A. PEPS construction

In this section we give a general PEPS construction, where matter and gauge degrees of freedom are associated with the vertices and edges, respectively, of an arbitrary oriented[4] graph. Throughout we use standard graph theory definitions and notation, c.f. [54], which we summarize in Appendix A.

Definition V.1 (PEPS). Let $\Gamma = (V, E)$ be an oriented[4] graph with Hilbert spaces $\mathcal{H}_v$ and $\mathcal{V}_e$ assigned to every vertex $v \in V$ and edge $e \in E$, respectively. We define a collection of *PEPS tensors* on Γ to be tensors

$$A_v \in \bigotimes_{o \in E_v^o} \mathcal{V}_o \otimes \mathcal{H}_v \otimes \bigotimes_{t \in E_v^t} \mathcal{V}_t^* \tag{31}$$

associated with each $v \in V$. The corresponding state, simply referred to as *PEPS*, is defined to be

$$|\Psi_\Gamma(A)\rangle := \mathrm{tr}_E \bigotimes_{v \in V} A_v \in \bigotimes_{v \in V} \mathcal{H}_v, \tag{32}$$

where we use tr_E to denote tensor contraction over all Hilbert spaces labeled by edges.

The Hilbert spaces denoted by $\mathcal{H}$ are referred to as *physical*, while the Hilbert spaces denoted by $\mathcal{V}$, introduced only for the purpose of constructing the PEPS, are referred to as *virtual*. As indicated by the notation, when we speak of a PEPS $|\Psi_\Gamma(A)\rangle$, we have implicitly fixed a collection of PEPS tensors giving rise to said state.

Definition V.2 (Global symmetry). We say a PEPS $|\Psi_\Gamma(A)\rangle$ has a *global symmetry*, or is *globally symmetric*, with respect to given representations $(\mathcal{H}_v, U_v) \in \mathrm{Rep}\,G$, for all $v \in \mathrm{vert}\,\Gamma$, if it satisfies

$$\bigotimes_{v \in \Gamma} U_v(g) |\Psi_\Gamma(A)\rangle = |\Psi_\Gamma(A)\rangle, \tag{33}$$

for all $g \in G$.

Definition V.3 (Local symmetry). We say a PEPS $|\Psi_\Gamma(A)\rangle$ has a *local symmetry*, or is *locally symmetric*, with respect to given representations $(\mathcal{H}_v, U_v) \in \mathrm{Rep}\,G$, for all $v \in \mathrm{vert}\,\Gamma$, if it satisfies

$$U_v(g) |\Psi_\Gamma(A)\rangle = |\Psi_\Gamma(A)\rangle, \tag{34}$$

for all $g \in G$ and $v \in \mathrm{vert}\,\Gamma$.

Clearly, the above definitions makes sense for any state in $\bigotimes_v \mathcal{H}_v$, not just PEPS. We introduce these terms to explicitly distinguish them from gauge-invariant PEPS, which are introduced later.

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[4] A graph is said to be oriented if it has no double edges or loops and each edge is given an orientation.

Definition V.4 (Blocking)**.** Let $|\Psi_\Gamma(A)\rangle$ be a PEPS and $\Gamma' = (V', E') \subseteq \Gamma$ a subgraph. The tensor

$$\mathbb{T}_{\Gamma'}(A) := \mathrm{tr}_{E'} \bigotimes_{v \in V'} A_v, \qquad (35)$$

where $\mathrm{tr}_{E'}$ denotes tensor contraction over all Hilbert spaces labeled by edges in E', is called *blocked PEPS tensor along* Γ'. The tensor $\mathbb{T}_{\Gamma'}(A)$ is said to be *injective* if it is injective as a map

$$\bigotimes_{e \in \partial_o \Gamma'} \mathcal{V}_e^* \otimes \bigotimes_{f \in \partial_i \Gamma'} \mathcal{V}_f^* \otimes \mathcal{V}_f \otimes \bigotimes_{d \in \partial_t \Gamma'} \mathcal{V}_d \longrightarrow \bigotimes_{v \in V'} \mathcal{H}_v, \ (36)$$

where $\partial_t \Gamma'$, $\partial_o \Gamma'$ and $\partial_i \Gamma'$ denote the terminal, original and internal boundaries[5] of Γ', respectively. In this context we will often say that Γ' defines an *injective region*.

Commonly one considers blocking along a full[6] subgraph, which simplifies the injectivity condition on the blocked tensor, since full subgraphs have empty internal boundary. Notice that for the special case where we choose a single vertex as the subgraph, the above notion of injectivity reduces to the usual one.

Rephrasing [51, Lemma 4] in the language of PEPS defined on oriented graphs gives the following useful lemma.

Lemma V.1 (Union of injective regions is injective)**.** Let $|\Psi_\Gamma(A)\rangle$ be a PEPS and $\Gamma_1, \Gamma_2 \subseteq \Gamma$ injective regions, i.e. the tensors $\mathbb{T}_{\Gamma_1}(A)$ and $\mathbb{T}_{\Gamma_2}(A)$ are injective. Then the union of the two subgraphs also defines an injective region, i.e. the blocked tensor $\mathbb{T}_{\Gamma_1 \cup \Gamma_2}(A)$ is injective.

Recall that in the example of Section III, we considered a square lattice, where we assigned physical Hilbert spaces and rank 3 tensors also to the edges of the lattice, which is the accepted way to define gauge theories on a lattice. In our general setting of PEPS defined on graphs, we only want to associate virtual Hilbert spaces with edges, hence it is most natural to introduce an additional vertex at each edge, resulting in the bipartite graph $\Gamma_b = (V, E, \mathcal{E})$, and carrying out the PEPS construction for Γ_b.

Definition V.5 (gPEPS)**.** The special case of a PEPS defined on $\Gamma_b = (V, E, \mathcal{E})$, the barycentric[7] subdivision of the oriented graph $\Gamma = (V, E)$, we call *gPEPS on* Γ. To reflect the bipartition of Γ_b we adopt slightly modified notation for the PEPS tensors

$$B_e \in \mathcal{V}_{e^t} \otimes \mathcal{H}_e \otimes \mathcal{V}_{e^o}^* \qquad (37)$$

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[5] The terminal (original) boundary is comprised of all incoming (outgoing) edges, c.f. Definition A.6.

[6] A full subgraph contains all edges in E connecting vertices in V', c.f. Definition A.5.

[7] The barycentric subdivision is obtained by inserting an additional vertex in the middle of each edge, resulting in the new set of edges $\mathcal{E}$, c.f. Definition A.9.

that are labeled by vertices in E, where e^o and e^t, defined in Equations (60), can be thought of as "half edges" of the original graph, and for the corresponding state

$$|\Psi_\Gamma(A, B)\rangle \in \bigotimes_{v \in V} \mathcal{H}_v \otimes \bigotimes_{e \in E} \mathcal{H}_e. \qquad (38)$$

To wit, given a graph $\Gamma = (V, E)$ we have associated to each vertex $v \in V$ a Hilbert space $\mathcal{H}_v$, which we think of as describing matter degrees of freedom, and to each edge $e \in E$ a Hilbert space $\mathcal{H}_e$, describing gauge degrees of freedom. We use the notation

$$\mathcal{H}^m := \bigotimes_{v \in V} \mathcal{H}_v, \qquad \mathcal{H}^g := \bigotimes_{e \in E} \mathcal{H}_e, \qquad (39)$$

for collectively referring to all matter (resp. gauge) degrees of freedom. The general PEPS construction, applied to Γ_b, then yields

$$A_v \in \bigotimes_{o \in \mathcal{E}_v^o} \mathcal{V}_o \otimes \mathcal{H}_v \otimes \bigotimes_{t \in \mathcal{E}_v^t} \mathcal{V}_t^*, \qquad (40)$$

$$B_e \in \mathcal{V}_{e^t} \otimes \mathcal{H}_e \otimes \mathcal{V}_{e^o}^*, \qquad (41)$$

for each $v \in V$ and $e \in E$. When comparing (41) with Equation (2), keep in mind that e^t originates at e while e^o terminates at e. We will sometimes refer to the tensors A and B as *vertex tensors* and *edge tensors*, respectively.

Definition V.6 (Gauge-invariant PEPS)**.** A gPEPS $|\Psi_\Gamma(A, B)\rangle$ is said to be *gauge-invariant*, referred to as *gauge-invariant PEPS* below, with respect to given representations $(\mathcal{H}_v, U_v), (\mathcal{H}_e, L_e), (\mathcal{H}_e, R_e) \in \mathrm{Rep}\, G$, for all $v \in V$ and $e \in E$, if

$$\widehat{U}_v(g) |\Psi_\Gamma(A, B)\rangle = |\Psi_\Gamma(A, B)\rangle, \qquad (42)$$

for all $g \in G$ and $v \in V$, where

$$\widehat{U}_v := \bigotimes_{e \in E_v^o} R_e \otimes U_v \otimes \bigotimes_{e \in E_v^t} L_e, \qquad (43)$$

is called *gauge operator centered at* v.

When we speak of a gauge-invariant PEPS $|\Psi_\Gamma(A, B)\rangle$, we will often leave the defining group representations implicit.

B. Main theorem

We prove that under mild assumptions the local tensors defining a gauge-invariant PEPS have to satisfy intertwiner relations analogous to the ones encountered in the square lattice example.

Definition V.7 (Invertible neighborhoods)**.** Let $|\Psi_\Gamma(A, B)\rangle$ be a gauge-invariant PEPS. We say that

$e \in \operatorname{edge}\Gamma$ has *invertible neighborhoods*,[8] if there are two disjoint subgraphs $\Lambda^\mathrm{o}, \Lambda^\mathrm{t} \subseteq \Gamma_\mathrm{b} \setminus \{e\}$, with $\mathrm{o}(e) \in \operatorname{vert}\Lambda^\mathrm{o}$ and $\mathrm{t}(e) \in \operatorname{vert}\Lambda^\mathrm{t}$, such that the blocked tensors $\mathbb{T}_{\Lambda^\mathrm{o}}(A,B)$ and $\mathbb{T}_{\Lambda^\mathrm{t}}(A,B)$ are injective.

Theorem V.1. Let $|\Psi_\Gamma(A,B)\rangle$ be a gauge-invariant PEPS. If $e \in \operatorname{edge}\Gamma$ has invertible neighborhoods, then there exist linear representations $(\mathcal{V}_{e^\mathrm{o}}, V_{e^\mathrm{o}}), (\mathcal{V}_{e^\mathrm{t}}, V_{e^\mathrm{t}}) \in \operatorname{Rep}G$, such that the corresponding edge tensor B_e satisfies the intertwiner relations

$$\quad , \quad (44)$$

for all $g \in G$.

Proof. Without loss of generality we may assume that the subgraphs Λ^t and Λ^o, defining the invertible neighborhoods, are full, connected and contain all vertices in $\Gamma_\mathrm{b} \setminus \{e\}$ adjacent to $\mathrm{t}(e)$ and $\mathrm{o}(e)$, respectively. We sketch an example of the general situation in Figure 3. Let J denote the set of all vertices in $\Gamma_\mathrm{b} \setminus \{e\}$ not included in Λ^t or Λ^o and let $\Lambda^\mathrm{j} := \Gamma_\mathrm{b}[J] \subseteq \Gamma_\mathrm{b}$ be the full subgraph induced by the set J. For brevity we drop the explicit dependence of the blocked tensors on the PEPS tensors from our notation. Let S be the set of edges in Γ_b not included in any of Λ^t, Λ^o or Λ^j, then we have

$$|\Psi_\Gamma(A,B)\rangle = \operatorname{tr}_S\left(\mathbb{T}_{\Lambda^\mathrm{t}} \otimes B_e \otimes \mathbb{T}_{\Lambda^\mathrm{o}} \otimes \mathbb{T}_{\Lambda^\mathrm{j}}\right)$$

$$= \qquad , \qquad (45)$$

where we do not draw the (generally numerous) physical legs of $\mathbb{T}_{\Lambda^\mathrm{j}}$. The blocked tensors $\mathbb{T}_{\Lambda^\mathrm{o}}$ and $\mathbb{T}_{\Lambda^\mathrm{t}}$ associated with the invertible neighborhoods are injective by assumption and the symmetry properties

$$\widehat{U}_{\mathrm{t}(e)}|\Psi_\Gamma(A,B)\rangle = \widehat{U}_{\mathrm{o}(e)}|\Psi_\Gamma(A,B)\rangle = |\Psi_\Gamma(A,B)\rangle \quad (46)$$

translate to

$$\qquad , \qquad (47)$$

where $\widetilde{U}_\mathrm{t}(g) \otimes L_e(g) := \widehat{U}_{\mathrm{t}(e)}(g)$ and

$$\qquad , \qquad (48)$$

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[8] Not to be confused with the neighbourhood of a vertex, which has a different meaning in graph theory.
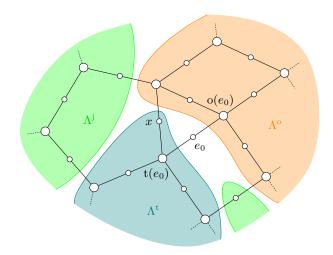

Figure 3. It is convenient to think of the graph Γ_b as being embedded in Euclidean space and label subgraphs by the spatial regions they are contained in. Since the edge tensors are all assumed to be LRI, whether the vertex x is seen as belonging to the orange or the teal region does not influence the injectivity of the blocked tensors associated with either subgraph. Only because the gauge operator centered at $\mathrm{t}(e_0)$ will also act on the degrees of freedom associated with x are we forced to include it in the teal region.

where $R_e(g) \otimes \widetilde{U}_\mathrm{o}(g) := \widehat{U}_{\mathrm{o}(e)}(g)$, hence the Fundamental Lemma IV.1 gives the claimed intertwiner properties. $\square$

Theorem V.2. Let $|\Psi_\Gamma(A,B)\rangle$ be a gauge-invariant PEPS on $\Gamma = (V,E)$. If all edges of Γ, with vertex $v \in V$ as an endpoint, have invertible neighborhoods, then the vertex tensor A_v will satisfy the intertwiner property

$$U_v(g) \circ A_v = A_v \circ \bigotimes_{f \in E_v^\mathrm{o}} V_{f^\mathrm{o}}^{-1}(g) \otimes \bigotimes_{e \in E_v^\mathrm{t}} V_{e^\mathrm{t}}(g), \quad (49)$$

for all $g \in G$, where $\{(\mathcal{V},V)\}$ are the representations of Theorem V.1 and we view A_v as a linear map

$$A_v : \bigotimes_{f \in E_v^\mathrm{o}} \mathcal{V}_{f^\mathrm{o}}^* \otimes \bigotimes_{e \in E_v^\mathrm{t}} \mathcal{V}_{e^\mathrm{t}} \longrightarrow \mathcal{H}_v. \quad (50)$$

Proof. By assumption, every $e \in E$ has invertible neighborhoods, which we shall respectively label Λ_e^t and Λ_e^o. Let $v_0 \in V$ and use the invertible neighborhoods of the surrounding edges to construct the subgraph

$$\Lambda_{v_0} := \bigcup_{e \in E_{v_0}^\mathrm{t}} \Lambda_e^\mathrm{o} \cup \bigcup_{f \in E_{v_0}^\mathrm{o}} \Lambda_f^\mathrm{t} \subseteq \Gamma_\mathrm{b}. \quad (51)$$

According to Lemma V.1, the blocked tensor $\mathbb{T}_{\Lambda_{v_0}}(A,B)$ is injective and since Λ_{v_0} contains all vertices adjacent to v_0 in Γ, the condition

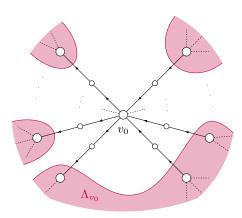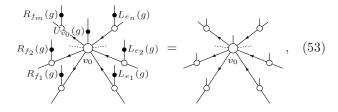$$\widehat{U}_{v_0}(g)|\Psi_\Gamma(A,B)\rangle = |\Psi_\Gamma(A,B)\rangle \quad (52)$$

Figure 4. We sketch a general example of how Λ_{v_0} looks like. While the individual invertible neighborhoods of the edges can be chosen to be full and connected, there is no reason why their union should remain to be so. Crucially, Λ_{v_0} contains all vertices adjacent to v_0 as a vertex of Γ, but none as a vertex of Γ_b.

is equivalent (by inverting $\mathbb{T}_{\Lambda_{v_0}}$ and tracing out the remaining degrees of freedom) to the equality

where $E_{v_0}^t = \{e_1, \ldots, e_n\}$ and $E_{v_0}^o = \{f_1, \ldots, f_m\}$. After using Theorem V.1 to move the representations R and L to the virtual legs and inverting the edge tensors, which are assumed to be LRI, we are left with

Corollary V.1. Let $|\Psi_\Gamma(A)\rangle$ be a normal PEPS on a *big enough* graph Γ and B_e be an arbitrary collection of unital edge tensors, such that the resulting gPEPS $|\Psi_\Gamma(A, B)\rangle$ is gauge-invariant. Then all vertex and edge tensors satisfy their appropriate intertwiner relations.

Proof. Big enough means that the injective regions, which can be constructed for each edge by the normality of the vertex tensors, do not overlap and form injective neighborhoods in the sense of V.7. Then the conditions of Theorem V.2 are satisfied for every vertex and the intertwiner properties hold everywhere. □

Corollary V.2. Let $|\psi_\Gamma(A)\rangle$ be a normal PEPS with local onsite symmetry on a *big enough* graph Γ. Then the PEPS tensors A_v transform trivially under the symmetry, i.e.

$$U_v(g) \circ A_v = A_v, \tag{55}$$

for all $g \in G$ and $v \in \text{vert}\,\Gamma$.

Proof. The PEPS $|\psi_\Gamma(A)\rangle$ can be viewed as a gauge-invariant gPEPS $|\psi_{\Gamma_b}(A, B = \mathbb{1})\rangle$, with trivial edge tensors and Hilbert spaces. Since the edge tensors transform trivially, Theorem V.2 implies the same for the vertex tensors. □

VI. CONCLUSIONS AND OUTLOOK

In this work we have analyzed the internal structure of tensor network states with a local (gauge) symmetry. The results derived here are valid for any dimension and geometry, and in particular for three space dimensional cubic lattices. The main technical assumptions of this work are the LRI property of the edge tensors and the invertibility condition, c.f. Definition V.7, imposed on all edges.

How these conditions can be weakened, e.g., by using other notions of injectivity, like G-injectivity that in 2D results in topologically ordered PEPS [55], we leave for future works. Another interesting problem is the construction of parent Hamiltonians, possessing these PEPS as their unique ground states.

Appendices

A. GRAPHS

Definition A.1 (Directed graph). A *directed graph* is an ordered pair $\Gamma = (V, E)$ of sets V and $E \subseteq V \times V$. The elements of the set $\text{vert}\,\Gamma := V$ are called *vertices* and the elements of the set $\text{edge}\,\Gamma := E$, which are ordered pairs of vertices, are called *edges*. For any edge $e \equiv (v_1, v_2) \in E$ the vertex $\text{o}(e) := v_1 \in V$ is called the *origin* of e and the vertex $\text{t}(e) := v_2 \in V$ is called the *terminus* of e. For any vertex $v \in V$ let E_v^{o} denote the set of edges that have v as their origin (i.e. the outgoing edges), E_v^{t} denote the set of edges that have v as their terminus (i.e. the incoming edges) and E_v denote the set of all adjacent edges. In formulas these sets are given as

$$E_v^{\text{o}} := \{e \in E \mid v = \text{o}(e)\},$$
$$E_v^{\text{t}} := \{e \in E \mid v = \text{t}(e)\},$$
$$E_v := E_v^{\text{o}} \cup E_v^{\text{t}}.$$

Definition A.2 (Oriented graph). A directed graph Γ for which $(v_1, v_2) \in \text{edge}\,\Gamma$ implies $(v_2, v_1) \notin \text{edge}\,\Gamma$, is called *oriented graph*.

Definition A.3 (Subgraph). We say that the graph Γ' is a *subgraph* of the graph Γ, denoted by $\Gamma' \subseteq \Gamma$, if $\text{vert}\,\Gamma' \subseteq \text{vert}\,\Gamma$ and $\text{edge}\,\Gamma' \subseteq \text{edge}\,\Gamma$. Subgraphs are said to be *disjoint* if their vertex sets are disjoint.

Remark. Clearly any subgraph of an oriented graph will also be oriented. Given a graph Γ one can construct all subgraphs by taking subsets $V \subseteq \text{vert}\,\Gamma$ and $E \subseteq \text{edge}\,\Gamma$ satisfying $\text{o}(e), \text{t}(e) \in V$ for all $e \in E$.

Definition A.4 (Union of subgraphs). Let $\Gamma_1 = (V_1, E_1)$ and $\Gamma_2 = (V_2, E_2)$ be subgraphs of Γ. We define the union of Γ_1 with Γ_2 to be the subgraph

$$\Gamma_1 \cup \Gamma_2 := (V_1 \cup V_2, E_1 \cup E_2) \subseteq \Gamma. \qquad (56)$$

Definition A.5 (Induced subgraph). A subgraph $\Gamma' \subseteq \Gamma$ is called *induced* or *full* if it contains all edges in Γ connecting vertices in $\text{vert}\,\Gamma'$. It is often denoted $\Gamma[S]$, where $S := \text{vert}\,\Gamma' \subseteq \text{vert}\,\Gamma$.

Definition A.6 (Boundary of a subgraph). Given a subgraph $\Gamma' = (V', E') \subseteq \Gamma = (V, E)$, we define the *internal*, *terminal* and *original boundaries* of Γ' (with respect to Γ) to be

$$\partial_{\text{i}}\Gamma' := \{e \in E \setminus E' \mid \text{o}(e) \in V' \wedge \text{t}(e) \in V'\},$$
$$\partial_{\text{t}}\Gamma' := \{e \in E \setminus E' \mid \text{o}(e) \notin V' \wedge \text{t}(e) \in V'\},$$
$$\partial_{\text{o}}\Gamma' := \{e \in E \setminus E' \mid \text{o}(e) \in V' \wedge \text{t}(e) \notin V'\},$$

respectively.

Definition A.7 (Bipartite graph). If the vertex set V of a graph $\Gamma = (V, E)$ is the union of two disjoint subsets $V = V_1 \cup V_2$ and every edge in E connects a vertex in V_1 with one in V_2, then we say Γ is a *bipartite* graph and we commonly write $\Gamma = (V_1, V_2, E)$.

Definition A.8 (Subdivision). Let $\Gamma = (V, E)$ be an oriented graph. The *subdivision* of Γ with respect to an edge $e = (v_1, v_2) \in E$ is an oriented graph Γ_e defined by

$$\text{vert}\,\Gamma_e := V \cup \{e\} \qquad (57)$$
$$\text{edge}\,\Gamma_e := E \cup \{(v_1, e), (e, v_2)\} \setminus \{e\}. \qquad (58)$$

Remark. Intuitively, we cut an edge in half and introduce a new vertex at the cut. The orientation of the new edges is induced from the original edge. The new edges $e^{\text{o}} := (v_1, e)$ and $e^{\text{t}} := (e, v_2)$ can respectively be viewed as the first and second half of what used to be the edge e. Pictorially:

 (59)

Definition A.9 (Barycentric subdivision). Subdividing every edge of a graph Γ yields a new graph Γ_{b}, called the *barycentric* subdivision of Γ.

Remark. The barycentric subdivision of any graph $\Gamma = (V, E)$ is bipartite and it is convenient to write $\Gamma_{\text{b}} = (V, E, \mathcal{E})$, where

$$\mathcal{E} = \bigcup_{e \in E} \{e^{\text{o}}, e^{\text{t}}\}, \quad e^{\text{t}} := (e, \text{t}(e)), \quad e^{\text{o}} := (\text{o}(e), e). \quad (60)$$

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