The minimal canonical form of a tensor network

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Abstract—Tensor networks have a gauge degree of freedom on the virtual degrees of freedom that are contracted. A canonical form is a choice of fixing this degree of freedom. For matrix product states, choosing a canonical form is a powerful tool, both for theoretical and numerical purposes. On the other hand, for tensor networks in dimension two or greater there is only limited understanding of the gauge symmetry. Here we introduce a new canonical form, the minimal canonical form, which applies to projected entangled pair states (PEPS) in any dimension, and prove a corresponding fundamental theorem. Already for matrix product states this gives a new canonical form, while in higher dimensions it is the first rigorous definition of a canonical form valid for any choice of tensor. We show that two tensors have the same minimal canonical forms if and only if they are gauge equivalent up to taking limits; moreover, this is the case if and only if they give the same quantum state for any geometry. In particular, this implies that the latter problem is decidable – in contrast to the well-known undecidability for equality of PEPS on grids. We also provide rigorous algorithms for computing minimal canonical forms. To achieve this we draw on geometric invariant theory and recent progress in theoretical computer science in non-commutative group optimization.

Index Terms—tensor networks, non-commutative optimization, invariant theory

1. INTRODUCTION

Tensor networks are a fruitful area of interconnection between quantum information theory, quantum many-body physics and computer science. On the one hand, tensor network states are rich enough to approximate with high accuracy most states which are relevant in condensed matter physics, such as Gibbs states and ground states. On the other hand, tensor networks are sufficiently simple that they enable one to manipulate complex quantum states, both numerically and theoretically. Tensor network representations of quantum states typically reduce the number of parameters describing the state from an exponential number to a number of parameters which is polynomial (or even constant) in the system size. For the purpose of numerics, one can then use this reduced parameter space to design variational optimization algorithms to simulate strongly interacting quantum systems. On the other side of the spectrum, tensor networks have been a powerful theoretical method to obtain simple characterizations of complex global quantum phenomena like topological order.

Roughly speaking, a tensor network is defined by a set of tensors with two types of indices: virtual ones, whose dimension is called the bond dimension, and physical ones, associated to the different subsystems of a quantum many-body system. These tensors generate a state (called a tensor network state) in the physical Hilbert spaces of the system by contracting the virtual indices on a given graph, typically a lattice associated to the interaction pattern of a Hamiltonian. The graphical notation for tensor network contractions is briefly reviewed in Fig. 1.

The success of tensor network states as a numerical variational family dates back to the pioneering paper [1], where...
the Density Matrix Renormalization Group (DMRG) algorithm was proposed as a way to approximate ground states of one-dimensional systems. Nowadays, this algorithm is seen as a way to minimize energy over the manifold of Matrix Product States (MPS), the first and most well-known family of tensor networks. From the perspective of quantum information theory, one may also see MPS as pairs of maximally entangled states to which locally a projection operator is applied. This allowed the generalization of the construction to more complex scenarios, including higher dimensions [2], [3]. There, the associated objects are called Projected Entangled Pair States (PEPS), precisely due to the perspective of applying projectors to a configuration of maximally entangled states. This construction of a two-dimensional PEPS tensor network is illustrated in Fig. 2. By now, there can be no doubt that this is one of the most important and powerful paradigms in numerical simulation of quantum systems [4]–[7], a recent highlight being the classical simulation [8] of the Google quantum supremacy experiment [9].

On the theoretical side tensor networks allow one to give local characterizations, in terms of their defining tensors, of global properties of interest, such as symmetries or topological order. The pioneering work [10], independently from the DMRG proposal [1], started this line of research. One of the first milestones was the cohomology-based classification of one-dimensional symmetry-protected topological (SPT) phases [11]–[13]. Today, this is an active area of investigation, see for instance the recent review [14] for details on the current state of the art. For instance, tensor networks are used for the characterization of topological order and topological phase transitions in higher spatial dimensions. Other important theoretical results concern rigorous approximation bounds, showing rigorously that classes of physically relevant states such as ground states and Gibbs states can be approximated accurately by PEPS.

Recently, due to their nice numerical and analytical properties, tensor networks have started to permeate other areas. In the context of physics notable examples are quantum gravity [15], [16] as well as (hybrid) classical simulation of quantum circuits [17], [18]. Outside of quantum physics, tensor networks have also attracted attention as a tool for machine learning [19]–[21] and as a (heuristic) tool for counting and optimization problems [22], [23].

The situation for spatially one-dimensional systems is qualitatively different from two or more spatial dimensions. In one spatial dimension, i.e. for MPS, there is both excellent understanding of the theoretical properties of MPS and their relation to one-dimensional many-body physics, as well as efficient algorithms for relevant computational tasks [14], [24], [25]. In two or more spatial dimensions the situation is markedly different and computational tasks associated to PEPS (such as computing the norm of the state) are known to be computationally hard [26]–[28]. Similarly, theoretical understanding of the structure of PEPS is much more limited [29]. As higher dimensional PEPS is clearly important for many-body systems as well as for simulation of quantum circuits it is important to further develop both the mathematical and algorithmic theory of PEPS.

An important feature both in theory and practice is the gauge symmetry of a tensor network. By inserting matrices on the virtual bonds of a tensor in such way that they cancel when the network is contracted, one modifies the local tensors while leaving the many-body state unchanged, see Fig. 3. In this context one desires: (1) a fundamental theorem that guarantees the gauge symmetry is the only freedom in tensors to give rise to the same states, and (2) a canonical form, which fixes this gauge degree of freedom in a natural way. Sometimes, both come together: some fundamental theorems only apply to tensors in a canonical form.

To make this more concrete, we consider PEPS in one spatial dimension, i.e., MPS. One key reason which make MPS easier to work with than, e.g., 2D PEPS, is that there are canonical forms with good theoretical properties and an associated fundamental theorem. This has played a crucial role in the development of the theory since its inception [10], see [14] for a review. We focus on the uniform (or translation-invariant) case, where one places the same 3-tensor $T$ on each site and contracts with periodic boundary conditions, resulting in a many-body quantum state $|T_n \rangle$ for any system size $n$. One may view $T$ as a tripartite quantum state on one physical and two virtual Hilbert spaces, the latter of bond dimension $D$. It is always possible (after blocking sites together and setting irrelevant off-diagonals to zero) to choose a gauge such that the reduced state on one of the two virtual Hilbert space is...
The result is called a left or right canonical form and it is unique up to unitary gauge symmetries. It has the following virtues:

(A) It satisfies a fundamental theorem: two tensors $T$ and $T'$ give rise to the same states on any number of sites, meaning $|T_n⟩ = |T'_n⟩$ for all $n$, if and only if they have a common canonical form.

(B) It allows lifting symmetries: if $T$ is in canonical form, any global symmetry $U^⊗n |T_n⟩ = |T'_n⟩$ for all $n$ can be implemented by a unitary gauge symmetry on $T$. This is key to classifying phases of matter and when studying entanglement spectra/Hamiltonians, to upgrade virtual to physical degrees of freedom.

(C) It provides a way to truncate, which is key for efficient accurate numerics: given a tensor $T$ with bond dimension $D$, it allows finding a tensor $T'$ which has bond dimension $D' < D$ such that $|T'_n⟩ ≈ |T_n⟩$ for all $n$. Clearly, it would be of great use to extend the theory of canonical forms to tensor networks in two or more spatial dimensions! However, it is known that there are significant obstructions. For example [28], [30]:

\begin{enumerate}
\item The following problem is undecidable: Given a PEPS tensor $T$, decide if the associated states $|T_{n,m}⟩$ vanish on periodic lattices of any size $n \times m$. This suggests there should not exist any useful (computable) canonical form generalizing (A), since by comparing the canonical forms of $T$ and the zero tensor one could otherwise decide whether $|T_{n,m}⟩ = 0$ for all $n$ and $m$. Indeed, before our work, no canonical form was known for PEPS tensor networks in two or more dimensions that applied to general tensors and rigorously satisfied properties such as the above.

On the other hand, a fundamental theorem is known if one restricts, e.g., to the class of normal tensors [31]. Moreover, heuristic approaches for canonical forms [32]–[36] and the truncation problem (C) are successfully used in practice to trade off computational efficiency and approximation accuracy [37].

A. Summary of results: a canonical form in any dimension and a fundamental theorem

In this work we introduce a new canonical form for general PEPS in arbitrary spatial dimension. It rigorously satisfies a number of desirable properties – particularly a fundamental theorem. The obstruction (i) is overcome by the following twist: roughly speaking, the canonical form captures when two tensors give rise to the same quantum states not just on the torus, but on any surface! This is achieved by pioneering the application of geometric invariant theory [38]–[40], an area of mathematics that studies group actions from the perspective of geometry and invariant theory, to the gauge symmetry of the tensor network and by drawing on recent theoretical computer science research on scaling problems and non-commutative group optimization.2 Scaling problems have been connected to a variety of interesting problems in mathematics and computer science, and can all be solved by minimizing the norm over an orbit in a representation of a well-behaved Lie group [51], [52]. Among them are the well-known matrix scaling [53], operator scaling [54] and tensor scaling problems [51]. Their study has led to a resolution of the Paulsen problem [55] and gives rise to efficient algorithms for non-commutative rational identity testing [56]. Other applications, to name a few, include an algorithmic solution to the quantum marginal problem [51], computing optimal constants for Brascamp-Lieb inequalities [57] and maximum-likelihood estimation in statistics [58], [59]. In this work, we identify a new application of this framework by relating it to the theory of canonical forms in tensor networks.

We now define the new canonical form and highlight its main properties and the new fundamental theorem. Here we only discuss uniform PEPS in $m$ spatial dimensions. These are defined by a single tensor $T$, with $2m + 1$ legs, one associated to the physical Hilbert space, and two legs each for the spatial directions $k \in \{1, \ldots, m\}$, associated with virtual Hilbert spaces of bond dimension $D_k$. The gauge group $G = GL(D_1) \times \cdots \times GL(D_m)$ acts on the virtual legs of the tensor as illustrated in Fig. 3. We say $T_{\text{min}}$ is a minimal canonical form of $T$ if it “infinizes” the $l_2$-norm among all gauge equivalent tensors:

\begin{equation}
T_{\text{min}} = \arg \min \|S\|_2 : S \in G \cdot T .
\end{equation}

Two important remarks are in order: First, consider the closure $\overline{G \cdot T}$ of the gauge group orbit of $T$, so that the minimum is attained. Thus there need not be a single gauge

As we will see in Definition III.5, strictly speaking this is only true independently in each of the diagonal blocks which remain in the canonical form. There is a proportionality constant that can be different in each one of those blocks.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2.png}
\caption{Uniform PEPS in 2D: A tensor $T$ gives rise to states $|T_{n,m}⟩$ on a periodic $n \times m$ lattice by placing $T$ at the sites and contracting with periodic boundary conditions.}
\end{figure}

\[330\]
Moreover, two tensors coincide with the usual ones for MPS (as if and only if \( \rho_T = \rho_{T'} \)). Following this characterization, illustrated in Fig. 4, the two virtual bonds in the tensor \( T \) as a (not necessarily normalized) quantum state, and we let the reduced states of the virtual bonds. To this end, interpret the condition as Corollary IV.9.

Guarantees the analogue of property (B) for normal tensors, that this is captured by the minimal canonical form. It also as Theorem III.9 for MPS and Theorem IV.7 for PEPS, states that global symmetries of the states \( |T_n, m\rangle \) can be lifted to \( |T'_n, m\rangle \) for all contraction graphs \( \Gamma \). It suffices to consider to graphs on \( e^{O(mD^3)} \) vertices.

We further show \( e^{O(mD)} \) vertices are necessary when \( m \geq 2 \) in Proposition IV.15, while for \( m = 1 \) we find two MPS tensors to be gauge equivalent iff \( |T_n\rangle = |T'_n\rangle \) for \( 1 \leq n \leq O(D) \), which is essentially tight [60]. Note that gauge equivalence is the same as having a common canonical form (by Result 1), and our fundamental theorem gives an important alternative characterization of this condition. Accordingly, our theorem proves a version of property (A) for PEPS in any spatial dimension, and as we show in Corollary IV.14, this also implies that global symmetries of the states \( |T_n\rangle \) can be lifted to unitary gauge symmetries, as in property (B). Strikingly, it also shows that deciding whether two tensors generate the same uniform PEPS \( |T_n\rangle \) on arbitrary contraction graphs is decidable – in stark contrast to the problem when we restrict to uniform PEPS \( |T_{n,m}\rangle \) on periodic rectangular lattices. The

Figure 3. Gauge invariance: For \( g = (g_1, g_2) \in GL(D_1) \times GL(D_2) \), if one defines the tensor \( S = g \cdot T \) as in the figure, the corresponding states \( |T_{n,m}\rangle \) and \( |S_{n,m}\rangle \) are equal.

Figure 4. Canonical form conditions: A tensor is in canonical form if the reduced density matrices of the tensor as a quantum state are equal up to transposition (corresponding to reversing the arrows in diagrammatic notation).
Result 2. We say that two tensors \( T \) and \( S \) are gauge equivalent, meaning \( G \cdot T \cap G \cdot S \neq \emptyset \) or that \( \lim_{m \to \infty} g^{(m)} \cdot T = \lim_{m \to \infty} h^{(m)} \cdot S \) for certain \( g^{(m)}, h^{(m)} \in G \) (equivalently, the two tensors have a common minimal canonical form), if and only if they contract to the same state on all contraction graphs.

On the other hand, it is undecidable to take the minimal canonical form, if and only if they contract to the same state on all contraction graphs.

Fundamental theorem: Two tensors \( S \) and \( T \) are gauge equivalent, meaning \( G \cdot T \cap G \cdot S \neq \emptyset \) or that \( \lim_{m \to \infty} g^{(m)} \cdot T = \lim_{m \to \infty} h^{(m)} \cdot S \) for certain \( g^{(m)}, h^{(m)} \in G \) (equivalently, the two tensors have a common minimal canonical form), if and only if they contract to the same state on all contraction graphs.

Figure 5. **Fundamental theorem:** Two tensors \( S \) and \( T \) are gauge equivalent, meaning \( G \cdot T \cap G \cdot S \neq \emptyset \) or that \( \lim_{m \to \infty} g^{(m)} \cdot T = \lim_{m \to \infty} h^{(m)} \cdot S \) for certain \( g^{(m)}, h^{(m)} \in G \) (equivalently, the two tensors have a common minimal canonical form), if and only if they contract to the same state on all contraction graphs.

B. Overview of methods: geometric invariant theory and geodesic convex optimization

On a high level, our approach is to start with the desired gauge symmetry and explore its natural consequences (rather than with a specific class of networks, such as PEPS on a torus). Geometric invariant theory (GIT) is a field of mathematics that studies group actions such as the above from the perspective of geometry and invariants [39], [40]. In general, given a group \( G \) and an action of \( G \) on a vector space \( V \), one studies the orbit

\[ G \cdot v = \{ g \cdot v : g \in G \} \]

and the orbit closure \( \overline{G \cdot v} \). In our case this means starting with the gauge group \( G = \text{GL}(D_1) \times \cdots \times \text{GL}(D_m) \) which acts on the vector space of PEPS tensors, which are tensors with dimensions \( (D_1, D_1, \ldots, D_m, D_m, d) \) and with the group action as shown in Fig. 3. To find a canonical form for a tensor \( T \), we wish to identify a special element in the orbit closure \( G \cdot T \). Minimum norm tensors provide a natural candidate.

We prove Results 1 and 2 by relying on the Kempf-Ness theorem [38], a fundamental result in GIT that studies minimum norm vectors in orbit closures. It states that minimum norm vectors in an orbit closure are unique up to the action by a maximal compact subgroup (which is \( U(D_1) \times \cdots \times U(D_m) \) for us), and that a vector \( v \in V \) is a minimal norm vector in the orbit closure \( G \cdot v \) if and only if

\[ \partial_{t=0} \| e^{tX} \cdot v \|^2 = 0 \]

for all \( X \) in the Lie algebra of \( G \). This condition translates to the condition in Result 2.

So far, we have focused on geometry, but we now move to invariants to connect to tensor networks and sketch the proof of our fundamental theorem in Result 3. A theorem by Mumford [39] implies that two tensors \( T, T' \) are gauge equivalent (meaning \( G \cdot T \cap G \cdot T' \neq \emptyset \)) if and only if \( P(T) = P(T') \) for any \( G \)-invariant polynomial \( P \). Now, for any contraction graph \( \Gamma \), the tensor network state \( |T_{\Gamma} \rangle \) is unchanged by gauge symmetries, and therefore its coefficients are \( G \)-invariant polynomials in \( T \). We use constructive invariant theory to prove that, conversely, any \( G \)-invariant polynomial can be obtained from coefficients of tensor network states. A theorem by Derksen [61] allows bounding the size of \( \Gamma \), which concludes the proof of Result 3. In Proposition IV.15 we also give an explicit construction for \( m \geq 2 \) of a tensor \( T \) which is such that its contraction \( |T_{\Gamma} \rangle \) on any contraction graph \( \Gamma \) with a number of vertices smaller than a bound exponential in \( D \) is zero, while for a larger number of vertices it can be nonzero. This implies that the required size of the contraction graph in Result 3 is exponential in \( D \) in general.

Next, for computational purposes we observe that computing

\[ T_{\min} = \text{arg min} \left\{ \|S\|_2 : S \in G \cdot T \right\} \]
is a non-commutative (group) optimization problem of the kind that has recently been of great interest in theoretical computer science [51], [52], [54], [55], [57], [62], [63]. While non-convex in the usual sense, such problems are geodesically convex, meaning the objective is convex along geodesics (shortest paths) of the domain. To prove Result 4, we instantiate the general framework of [52]. This provides first and second order optimization algorithms, where the runtime of the algorithms is determined by representation theoretic data associated to the Lie group and the representation of interest. The first algorithm in Result 4 is a first order algorithm, performing geodesic gradient descent. The second algorithm in Result 4 is a second order algorithm, which also uses information about the second derivatives (the Hessian) of the objective function. We compute the representation theoretic data (the weight margin and the weight norm) required to apply the framework of [52] in the specific case of $G = \text{GL}(D_1) \times \cdots \times \text{GL}(D_m)$, acting on the space of PEPS tensors. The natural error measure in the framework of [52] is to bound the error in the first-order characterization as in Eq. (I.3), rather than the error in the space of tensors as in Eq. (I.2). Our main technical contribution here is Theorem V.14, which extends an approach of [55] to bound the error in the space of tensors using the error in the first-order characterization and the weight margin. This argument generalizes readily to other scaling algorithms and is of independent interest.

C. Conclusions and outlook

The main contribution of our work is to show that geometric invariant theory yields a natural approach to defining canonical forms for tensor networks. Given the practical and theoretical importance of canonical forms and fundamental theorems, we hope our results offer a useful new tool for the study and application of tensor networks, and our work may be a starting point for a fruitful application of methods in invariant theory and non-commutative optimization to tensor networks. To highlight the power of these tools we note that even in the MPS case our approach leads to a canonical form in a particularly elegant way. In previous work (for instance [64]) special care had to be taken in order to deal with certain off-diagonal terms when constructing canonical forms. This is resolved in a natural way by extending the notion of gauge equivalence to the closure of the gauge group orbit. For PEPS with $m \geq 2$ before our work no rigorous results for canonical forms for general tensors were known, and we show the existence of a canonical form together with a fundamental theorem. Finally, the problem of computing the minimal canonical form is an instance of a non-commutative optimization problem, and we provide an important new application of the broader framework of non-commutative optimization that has been of significant recent interest.

Let us briefly discuss some potential applications and extensions of our results. We have proven a fundamental theorem, which was application (A). From a many-body theory perspective, our results may be helpful in studying virtual symmetries of tensor networks as in application (B), which are crucial in understanding topological order. From a practical perspective, it would be interesting to investigate if our canonical form can improve the numerical stability of variational optimization algorithms and other numerical methods [65], as it could be expected by the known close connection between gauge fixing and stability [35], [66]. Another important practical application would be to investigate whether the minimal canonical form provides a useful way to truncate bond dimensions as in (C).

Our results also imply that one can sample uniformly from all PEPS tensors in minimal canonical form in the same orbit. This has applications beyond quantum information, e.g., it allows to extend the technique of [67] for enhancing privacy in machine learning from MPS to PEPS. Our approach generalizes naturally to other tensor network types and gauge groups, and exploring this is an exciting direction for future work. Of particular interest is the non-uniform case where we have different tensors at each site. For the MPS case we can indeed relate our framework to known canonical forms (see Section III-C). Finally, there are a number of interesting algorithmic questions. One such question is to find (efficient) algorithms for deciding gauge equivalence. Our fundamental theorem, Result 3 allows one to check algorithmically whether $T$ and $S$ are gauge equivalent, simply by checking equivalence on all contraction graphs up to some exponential size. Another approach would be to compare the minimal canonical forms. While we provide algorithms to compute the minimal canonical form, there is still a remaining unitary group action, and it would be interesting to find an algorithm which determines unitary equivalence (which is known in the case $m = 1$). We discuss all these points further in Section VI.

D. Organization of the paper

We start in Section II by reviewing basic results from geometric invariant theory in a general setting. Then we apply this to construct the minimal canonical form for MPS in Section III. Our main results are stated in Section IV, where we introduce the minimal canonical form for PEPS and prove its basic properties. In Section V we provide algorithms for computing the minimal canonical form and relate to recent work on non-commutative optimization. We end with a brief outlook in Section VI, suggesting applications for the minimal canonical form and avenues for future research.

Notation

We let $[k] := \{1, \ldots, k\}$ and denote by $\mathbb{C}^*$ the nonzero complex numbers. We write $y = \arg \min_{x} {f(x) : x \in X}$ to denote that $y \in X$ and $f(y) = \min_{x} {f(x) : x \in X}$; in general this will not uniquely determine $y$. Throughout we write $\langle \cdot, \cdot \rangle$ for inner products and $\|\cdot\|_2$ for the corresponding Euclidean or $\ell^2$-norm. We write Mat$_{n,n'}$ for the complex vector space of complex $n \times n'$ matrices and Herm$_n$ for the real vector space of Hermitian $n \times n$ matrices, which we will always endow with the Hilbert-Schmidt inner product $\langle A, B \rangle := \text{tr}[A^\dagger B]$. Thus, $\|A\|_2 := \sqrt{\langle A, A \rangle}$ denotes the Hilbert-Schmidt (or Frobenius or Schatten-2) norm of a matrix $A \in \text{Mat}_{n,n'}$. We will (very
We write which we denote by $\|A\|_\infty$. We denote identity matrices by $I$ and use subscripts to denote context when this increases clarity. We write $\GL(n)$ for the general linear group, which consists of the invertible $n \times n$ matrices, and $\SL(n)$ for the special linear group, which consists of the $n \times n$ matrices of unit determinant. We will use boldface for $m$-tuples of matrices, e.g., $X = (X_1, \ldots, X_m)$ (as well as similarly in the case of open boundary conditions in Section III-C), but never for the $d$-tuples that make up uniform MPS or PEPS tensors. Finally, we denote by $\mathbb{C}[V]$ the algebra of polynomial functions on a vector space $V$.

II. PRELIMINARIES IN GEOMETRIC INVARIANT THEORY

Geometric invariant theory (GIT) is a field of mathematics that studies orbits of group actions from a perspective that combines geometry and algebra. In this section we give a gentle introduction to this theory and review some central results. In subsequent sections we will apply it to define and analyze our new canonical form for tensor networks. A good reference on GIT is the textbook by Wallach [40] and we follow his concrete approach; for a more abstract account see the seminal monograph [39].

Throughout this section, we fix a subgroup $G \subseteq \GL(n)$ that is closed under taking adjoints, i.e., $g^\dagger \in G$ for every $g \in G$. We furthermore assume that $G$ is defined by polynomial equations, i.e., $G = \{g \in \GL(n) : P_i(g) = 0 \text{ for all } i \in [k]\}$ for certain polynomials $P_1, \ldots, P_k$ in the matrix entries of $g$. The unitary matrices in $G$ form a maximally compact subgroup, which we denote by $K = G \cap \U(n)$.

Example II.1. We will almost exclusively deal with groups of the form $G = \GL(D_1) \times \cdots \times \GL(D_m)$. These can be realized as above as the subgroup of $\GL(n)$, $n = D_1 + \cdots + D_m$, consisting of block diagonal invertible matrices with blocks of size $D_k \times D_k$ for $k \in [m]$. Then $K = \U(D_1) \times \cdots \times \U(D_m)$.

Next, we fix a representation $\pi: G \to \GL(V)$ on a finite-dimensional Hilbert space $V \cong \mathbb{C}^N$. Recall that $\pi$ is a representation if $\pi(1_G) = 1_V$ and $\pi(gh) = \pi(g)\pi(h)$ for all $g,h \in G$. We will assume that $\pi$ is regular or rational, meaning that the matrix entries of $\pi(g)$ with respect to any basis are polynomial functions of the matrix entries of $g$ and of $\det(g)^{-1}$. Finally, we assume that $\pi(K) \subseteq \U(V)$, meaning that the unitary matrices in the group act unitarily on the Hilbert space.

To emphasize that the group acts on vectors, we often write $g \cdot v := \pi(g)v$ for the action of a group element $g \in G$ on a vector $v \in V$. Then the orbit of a vector $v \in V$ is the set of all vectors that can be obtained by the group action, denoted $G \cdot v := \{g \cdot v : g \in G\}$. Since the group $G$ is never compact, orbits will in general not be closed; hence we will also be interested in the orbit closure $\overline{G \cdot v}$. One of the central goals of GIT is to classify vectors under the group action, and it is natural to allow taking limits, as we explained in the introduction in the context of PEPS. Thus, GIT is concerned with classifying orbit closures up to a natural notion of equivalence, where two vectors $v,v'$ are called equivalent if

$$\overline{G \cdot v} \cap \overline{G \cdot v'} \neq \emptyset.$$ 

To this end, one would like to pick out special points in orbit closures. Minimum norm vectors are natural candidates, generalizing Eq. (I.1). The following terminology is not standard, but natural:

Definition II.2 (Minimum norm vectors). For $v \in V$, we say that $v_{\text{min}}$ is a minimum norm vector for $v$ if

$$v_{\text{min}} = \arg \min \{\|w\|_2 : w \in \overline{G \cdot v}\}.$$ 

That is, $v_{\text{min}}$ is a minimum norm vector for $v$ if $v_{\text{min}} \in \overline{G \cdot v}$ and $\|v_{\text{min}}\|_2 = \min_{w \in \overline{G \cdot v}} \|w\|_2 = \inf_{g \in G} \|g \cdot v\|_2$.

Clearly, any vector $v$ has a minimum norm vector $v_{\text{min}}$. The latter is in general not unique, since if $v_{\text{min}}$ is a minimum norm vector then so is $k \cdot v_{\text{min}}$ for any $k \in K$ (recall that $K$ preserves the norm). Crucially, this is the only source of non-uniqueness. Moreover, two orbit closures intersect if and only if they have a common minimum norm vector! We summarize these fundamental results of GIT:

Theorem II.3. Let $v \in V$. Then minimum norm vectors for $v$ exist and form a single $K$-orbit (meaning that any two minimum norm vectors $w,w'$ satisfy $K \cdot w = K \cdot w'$). Moreover, if $v' \in V$, one has $\overline{G \cdot v} \cap \overline{G \cdot v'} \neq \emptyset$ if and only if $v$ and $v'$ have a common minimum norm vector.

We now focus on the properties of the minimum norm vector itself and give some intuition why Theorem II.3 holds. It is clear that if $w$ is a vector of minimal norm in an orbit closure, then it is in particular a vector of minimal norm in its own $G$-orbit, hence the derivatives of the norm (or norm squared) must vanish in any direction along the orbit.

What are these directions? They are given by the Lie algebra $\mathfrak{Lie}(G)$ of $G$, which is the complex vector space consisting of all matrices $X \in \Mat_{n \times n}$ such that $e^{tX} \in G$ for all $t \in \mathbb{R}$. Then $t \mapsto e^{tX} \cdot v$ is a smooth curve in the orbit of $w$. Accordingly, if $w$ is a vector of minimum norm in its orbit then $\|e^{tX} \cdot w\|_2^2$ must have a minimum at $t = 0$ and hence its derivative will vanish. This motivates the following definition:

Definition II.4. A vector $w \in V$ is called critical if $\partial_t|_{t=0} \|e^{tX} \cdot w\|_2^2 = 0$ for every $X \in \mathfrak{Lie}(G)$.

Since $K$ acts unitarily, the norm will always be preserved if we move in directions that keep us in the $K$-orbit. The latter are given by the Lie algebra $\mathfrak{Lie}(K)$ of $K$, which is defined analogously. One can show that Definition II.4 is equivalent

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3That is, $G$ is a Zariski-closed subgroup of $\GL(n)$ that is closed under taking adjoints. Such groups can also be defined more abstractly and are known as complex reductive algebraic groups.

4The closure can be taken with respect to the standard topology induced by the norm. For orbits, this coincides with the Zariski topology, and this is important for establishing the theory, but we will never need to use this explicitly.
to demanding that \( \partial_t v = 0 ||e^X v||^2 = 0 \) for all \( X \in i \text{Lie}(K) \); the latter are precisely the Hermitian matrices in \( \text{Lie}(G) \).

Criticality is the natural first-order condition for a vector to have minimum norm in its orbit ("at a minimum, all derivatives vanish"). Remarkably, this is also sufficient. This result is part of a key theorem by Kempf and Ness [38], which further characterizes the existence of minimum norm vectors:

**Theorem II.5 (Kempf–Ness).** Let \( v \in V \). Then:

1. \( v \) is critical if and only if \( ||g \cdot v||^2 \geq ||v||^2 \) for every \( g \in G \) (i.e., \( v \) has minimum norm in its orbit).
2. If \( v \) is critical and \( w \in G \cdot v \) is such that \( ||v||^2 = ||w||^2 \), then \( w \in K \cdot v \).
3. If \( G \cdot v \) is closed then there exists a critical element \( v' \in G \cdot v \).
4. If \( v \) is critical then \( G \cdot v \) is closed.

In particular, \( v \) is a minimum norm vector for itself (i.e., has minimum norm in \( G \cdot v \)) if and only if it has minimum norm in its orbit (meaning \( ||g \cdot v||^2 \geq ||v||^2 \) for all \( g \in G \)), which is the case if and only if \( v \) critical.

Thus, minimum norm vectors (or critical vectors) are unique up to the \( K \)-action, and they can be found precisely in closed \( G \)-orbits. While \( G \)-orbits are not closed in general, it is well-known that any orbit closure contains a unique closed orbit.

**Lemma II.6.** Every orbit closure \( G \cdot v \) contains a unique closed \( G \)-orbit.

Accordingly, the minimum norm vectors \( v_{\text{min}} \) for any vector \( v \in V \) are precisely the vectors of minimal norm in the unique closed orbit inside \( G \cdot v \). Theorem II.3 follows from this and the Kempf–Ness theorem. Indeed, the first claim in Theorem II.3 is immediate, and for the second claim we only need to argue that \( G \cdot v \cap G \cdot v' \neq \emptyset \) implies that the two vectors have a common minimum norm vector. To this end, take any \( v'' \in G \cdot v \cap G \cdot v' \).

Then \( G \cdot v \cap G \cdot v' \) contains \( G \cdot v'' \), which in turn contains a closed orbit. Thus both \( G \cdot v \) and \( G \cdot v' \) contain the same closed orbit, and hence \( v \) and \( v' \) have the same minimum norm vectors.

It is interesting to ask why Lemma II.6 is true. Even though so far we only discussed geometry, to answer this question we have to turn towards invariant theory.

**Definition II.7.** A \((G-)\)invariant polynomial is a polynomial \( P \in \mathbb{C}[V] \) such that, for every \( g \in G \) and \( v \in V \), \( P(g \cdot v) = P(v) \). The invariant ring, denoted \( \mathbb{C}[V]^G \), is the algebra consisting of all \( G \)-invariant polynomials.

Then the point is that any two closed orbits can be separated by a \( G \)-invariant polynomial.

**Lemma II.8.** Suppose that two orbits \( G \cdot v \) and \( G \cdot v' \) are closed and disjoint. Then there exists an invariant polynomial \( P \in \mathbb{C}[V]^G \) such that \( P(v) \neq P(v') \).

3As one might imagine the reason is a kind of convexity (in, as it turns out, a natural non-Euclidean geometry), and we will explain this in more detail in Section V.

This implies Lemma II.6 at once, since any \( G \)-invariant polynomial is a continuous function and hence constant not just on orbits but even on orbit closures. Furthermore, it implies the following important result, which connects geometry (orbit closures) and algebra (invariants):

**Theorem II.9 (Mumford).** Let \( v, v' \in V \). Then, \( G \cdot v \cap G \cdot v' \neq \emptyset \) if and only if \( P(v) = P(v') \) for all invariant polynomials \( P \in \mathbb{C}[V]^G \).

We end with a classical fact about invariant rings.

**Theorem II.10 (Hilbert finiteness).** The invariant ring \( \mathbb{C}[V]^G \) is a finitely generated algebra.

Moreover, there exist algorithms that compute generators \( P_1, \ldots, P_k \in \mathbb{C}[V]^G \) [68]. Accordingly, determining whether two vectors \( v, v' \) are equivalent in the sense of GIT (i.e., \( G \cdot v \cap G \cdot v' \neq \emptyset \) can in principle be decided by an algorithm – simply check whether \( P_i(v) = P_i(v') \) for all \( i \in [k] \). However, this is impractical, since known algorithms for computing generators are inefficient (run in exponential time or worse) and in many situations one will have to deal with generators that have exponentially large degree (we will in fact see an example in Section IV) or are hard to evaluate in the sense of computational complexity [69]. Moreover, it is not clear how such an algebraic approach could go beyond the decision problem to compute, e.g., minimum norm vectors. This motivates the search for alternative algorithms. We will return to this point in Section V, but first we discuss in Sections III and IV how the machinery of geometric invariant theory and in particular Theorems II.3 and II.9 allow defining new canonical forms for tensor networks that enjoy very good theoretical properties.

## III. Matrix Product States

In this section, we discuss the setting of matrix product states (MPS). While MPS are very well-understood theoretically, it is instructive to revisit this setting from our new perspective and contrast our minimal canonical form to the known ones, which also enjoy excellent theoretical properties.

We start by defining uniform (or translation-invariant) MPS and briefly reviewing existing canonical forms in Section III-A. We then introduce the minimal canonical form in Section III-B. Finally, in Section III-C we also discuss the case of non-uniform MPS with open boundary conditions.

### A. Gauge freedom and canonical forms for uniform MPS

We denote by \( \text{Mat}_D^{\times D} \) the vector space of \( D \times D \)-matrices.

**Definition III.1 (Uniform MPS).** For any matrix tuple \( M = (M^{(i)})_{i=1}^d \in \text{Mat}_D^{\times D} \) and system size \( n \in \mathbb{N} \), we define the uniform (or translation-invariant) matrix product state (MPS) as the (not necessarily) quantum state \( |M_n\rangle \in (\mathbb{C}^d)^{\otimes n} \) whose coefficients are given by

\[
\langle i_1, \ldots, i_n | M_n \rangle = \text{tr} M^{(i_1)} \cdots M^{(i_n)}
\]

for all \( i_1, \ldots, i_n \in [d] \). We refer to \( d \) as the physical dimension and \( D \) as the bond dimension.
We may then compute the reduced density matrices of \( \rho \) as an \( n \)-tuple gauge symmetry.

\[
\langle M \rangle = \langle g \cdot M \rangle,
\]

or as an (unnormalized) quantum state \( |M\rangle \). By definition, we define the gauge action \( \hat{M} \) on \( |M\rangle \) by

\[
\hat{M}|M\rangle = g\cdot M = (gMg^{-1})|M\rangle.
\]

We may then compute the reduced density matrices of \( \rho = |M\rangle \langle M| \) on either of the two virtual Hilbert spaces:

\[
\rho_1 = \sum_{i=1}^{d} M^{(i)}(M^{(i)})^\dagger \quad \text{and} \quad \rho_2 = \sum_{i=1}^{d} (M^{(i)})^\dagger M^{(i)}. \quad (\text{III.2})
\]

An important property of MPS is that the states \(|M_n\rangle\) are left invariant (for any \( n \)) if we conjugate each matrix \( M^{(i)} \) in the tuple by the same invertible matrix. Formally:

**Definition III.2** (Gauge action). We define the gauge action of \( g \in \text{GL}(D) \) on \( M = (M^{(i)})_{i=1}^{d} \) by

\[
g \cdot M := (gMg^{-1})|M\rangle.
\]

If we think of \( M \) as a quantum state \(|M\rangle\) in \( H_1 \otimes H_2 \otimes H_{\text{phys}} \), the gauge action can be written as

\[
g \cdot |M\rangle := |g\cdot M\rangle = (g \otimes g^{-T} \otimes I)|M\rangle.
\]

**Lemma III.3** (Gauge symmetry). For every \( M \in \text{Mat}^{d}_{D \times D} \), \( g \in \text{GL}(D) \), and \( n \in N \), we have

\[
|M_n\rangle = |(g \cdot M)_n\rangle.
\]

This is shown in Fig. 7.

It is then a natural question to ask whether this is the only freedom in the tensor \( M \) to define the same state \(|M_n\rangle\) for all \( n \). The answer is no, as is well-known and illustrated by the following example:

**Example III.4.** Let

\[
M^{(0)} = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad M^{(1)} = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}
\]

and

\[
\hat{M}^{(0)} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \hat{M}^{(1)} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.
\]

Then both tensors define the same MPS, for any system size \( n \in N \), namely the GHZ states

\[
|M_n\rangle = |\hat{M}_n\rangle = |0\rangle^\otimes n + |1\rangle^\otimes n.
\]

However, there is no \( g \in \text{GL}(D) \) so that \( g \cdot M = \hat{M} \).

The underlying problem is that when the matrices \( M^{(i)} \) in a tuple are all in upper triangular form (with respect to some basis), the off-diagonal terms are totally irrelevant for the final state \(|M_n\rangle\). The standard way to deal with this is to remove such off-diagonal terms in a structured manner. Let us briefly sketch the procedure, but refer to [14] and [70] for details and nomenclature.

One starts looking for a minimal common invariant subspace of all \( M^{(i)} \) and change \( M^{(i)} \) by \( PM^{(i)}P + QM^{(i)}Q \), with \( P \) being the orthogonal projector onto such a subspace and \( Q = I - P \). It is not difficult to see that this new tensor defines the same original MPS. Now one proceeds similarly with \( QM^{(i)}Q \) until one reaches a block diagonal form. The minimality of the subspaces guarantees that, in each of the diagonal blocks, the corresponding tensor, say \( M_{\text{phys}} \), fulfills the property that the associated completely positive (CP) map \( \mathcal{E}_b \) given by

\[
X_b \mapsto \sum_i M^{(i)}_b X_b (M^{(i)}_b)^\dagger
\]

is irreducible. Normalizing so that the spectral radius of the map is 1, this implies that the eigenvalues of modulus 1 are all non degenerate and they are exactly the \( q \)-th roots of unity with a \( q \) dividing the size \( D_b \) of the matrices \( M^{(i)}_b \). One can then distinguish two cases: \( q = 1 \), in which case the map \( \mathcal{E}_b \) is primitive, or \( q > 1 \), in which case one can “block” or group together \( q \) sites; then the resulting tensor in \( H_1 \otimes H_2 \otimes H_{\text{phys}}^{\otimes q} \) consists of block diagonal matrices whose associated CP maps are also primitive.

To make a long story short, starting with a matrix tuple \( M \), after projecting and blocking following the above procedure, one obtains a new matrix tuple \( \hat{M} \) such that at least \( \hat{M}^{(i)} \) is block diagonal, \( \hat{M}^{(i)} = \oplus_b M^{(i)}_b \), and the CP maps \( \mathcal{E}_b \) are all primitive. It is now possible to act with a gauge \( g \in \text{GL}(D) \), which can also be taken to be block-diagonal, \( g = \oplus_b g_b \), so that one obtains in each block \( b \) of \( \hat{M} := g \cdot \hat{M} \) the canonical condition. That is, there exist constants \( c_b \in \mathbb{R}_+ \) such that

\[
\sum_{i=1}^{d} (\hat{M}^{(i)}_b)^\dagger \hat{M}^{(i)}_b = c_b I_{D_b} \quad (\forall b), \quad (\text{III.3})
\]

meaning that, after normalization, the maps \( \mathcal{E}_b : X_b \mapsto \sum_i \hat{M}^{(i)}_b X_b (\hat{M}^{(i)}_b)^\dagger \) are trace preserving completely positive maps.
(TPCP) maps, i.e., quantum channels. One could analogously have taken the dual condition
\[ \sum_{i=1}^{d} \hat{M}_b^{(i)} (\hat{M}_b^{(i)})^\dagger = c_b I_{D_b} \quad (\forall b), \] (III.4)
meaning the \( E_b \) are completely positive unital (CPU) maps.

For generic matrix tuples \( M \), the channel defined by \( X \mapsto \sum_i M^{(i)} X (M^{(i)})^\dagger \) is already primitive. In this case, \( M \) is called normal and one can obtain a left or right canonical form \( M \) by acting with a suitable gauge group element: \( M = g \cdot M \) for some \( g \in \text{GL}(D) \).

**Definition III.5** (Left and right canonical form). A matrix tuple (MPS tensor) is said to be in left canonical form if it is block diagonal, with each diagonal block a normal tensor fulfilling Eq. (III.3). The right canonical form is defined analogously by imposing the dual condition in Eq. (III.4).

The above procedure guarantees that, after discarding off-diagonal blocks and at the price of blocking, one can bring any MPS tensor into left or right canonical form. For instance, in Example III.4 the tensor \( M \) is block diagonal, its blocks are 1-dimensional and hence trivially primitive, and moreover \( \hat{\rho}_1 = \hat{\rho}_2 = \hat{I}_2 \). Thus \( M \) is both in left and right canonical form. For tensors in canonical form, (unitary) gauge symmetry is the only freedom for two tensors to generate the same MPS.

**Theorem III.6** (Fundamental theorem of MPS, [14], [64]). Let \( M, N \) be both in left (or right) canonical form and \( |M_n\rangle = |N_n\rangle \) for all \( n \in \mathbb{N} \). Then there exists a unitary \( u \in U(D) \) such that \( u \cdot M = N \).

The name “fundamental theorem” stems from its numerous applications, and we refer for instance to [14] or [71] for an accounting of several of these.

**B. The minimal canonical form for uniform MPS**

We now define a new canonical form for uniform MPS. Its appeal is that it will naturally generalize to tensors with an arbitrary gauge symmetry and in particular to PEPS in higher dimensions, and that it can be analyzed using the powerful tools from geometric invariant theory.

Our starting point is the following simple but powerful observation: For a given matrix tuple \( M \in \text{Mat}_{D \times D}^d \), we should not only consider gauge transformations \( M \mapsto g \cdot M \) for some \( g \in \text{GL}(D) \), but also limits of such. Indeed, suppose we have a sequence of gauge group elements \( g_k \in \text{GL}(D) \) such that \( g_k \cdot M \) converges to some \( \hat{M} \). Then, since the MPS \( |M_n\rangle \) are continuous functions of the matrix tuple \( M \), we still have
\[ |\hat{M}_n\rangle = \lim_{k \to \infty} |(g_k \cdot M)_n\rangle = |M_n\rangle \quad (\forall n \in \mathbb{N}). \]

In other words, all matrix tuples in the orbit closure \( \text{GL}(D) \cdot M \) determine the same MPS. This naturally leads to the following definition:

**Definition III.7** (Gauge equivalence). Let \( M, N \in \text{Mat}_{D \times D}^d \) be two matrix tuples. We say that \( M \) and \( N \) are gauge equivalent if and only if \( \text{GL}(D) \cdot M \cap \text{GL}(D) \cdot N \neq \emptyset \).

This is the natural notion of gauge equivalence for MPS tensors, since if \( M \) and \( N \) are gauge equivalent in the sense just defined then
\[ |M_n\rangle = |N_n\rangle \quad (\forall n \in \mathbb{N}). \]

Indeed, it is the smallest equivalence relation generated by gauge transformations and taking limits. In particular, to define a canonical form we should naturally look at orbit closures, not just at orbits. How could we single out special elements in the orbit closure? Section II motivates the following definition:

**Definition III.8** (Minimal canonical form of MPS). We say \( M_{\text{min}} \in \text{Mat}_{D \times D}^d \) is a minimal canonical form for a matrix tuple (MPS tensor) \( M \in \text{Mat}_{D \times D}^d \) if it is an element of minimal norm in the orbit closure of the latter:
\[ M_{\text{min}} = \arg \min \{ \|M'\|_2 : M' \in \text{GL}(D) \cdot M \}, \]
where we use the Euclidean norm of \( M \) (or \( |M\rangle \)), that is,
\[ \|M\|_2 = \sqrt{\langle M | M \rangle} = \left( \sum_{i=1}^{d} \text{tr} \left( (M^{(i)})^\dagger M^{(i)} \right) \right)^{1/2} = \left( \text{tr} \left( \sum_{i=1}^{d} (M^{(i)})^\dagger M^{(i)} \right) \right)^{1/2}. \]

We say \( M \in \text{Mat}_{D \times D}^d \) is in minimal canonical form if it is a minimal canonical form for itself.

Note that any MPS tensor has a minimal canonical form – in contrast to the usual left or right canonical form of Definition III.5, no explicit projecting and blocking is required.

Clearly, the minimal canonical form is a special case of the general notion of a minimum norm vector (Definition II.2) for the action of \( G = \text{GL}(D) \) on \( V = \text{Mat}_{D \times D}^d \) (Definition III.2). We can now use the general theory of geometric invariant theory to understand the basic properties of this canonical form and we will see the usefulness of the general results of Section II. First of all, while the minimal canonical form is not uniquely defined, it is uniquely defined up to unitary gauge transformations (the action of \( K = U(D) \)), and it precisely characterizes gauge equivalence (Definition III.7):

**Theorem III.9** (Minimal canonical form). Let \( M, N \in \text{Mat}_{D \times D}^d \). Then the following are equivalent:
1. \( M \) and \( N \) have a common minimal canonical form.
2. If \( M_{\text{min}}, N_{\text{min}} \) are minimal canonical forms of \( M, N \) then \( U(D) \cdot M_{\text{min}} = U(D) \cdot N_{\text{min}} \). That is, minimal canonical forms of \( M \) and \( N \) are related by unitary gauge symmetries.
3. \( M \) and \( N \) are gauge equivalent, i.e., \( \text{GL}(D) \cdot M \cap \text{GL}(D) \cdot N \neq \emptyset \).

**Proof.** This is an immediate consequence of Theorem II.3. □
Theorem III.10 (Characterization) \( \rho \). Equivalently, the reduced density matrices of \( \hat{\rho} \) for a matrix tuple \( M \in \text{Mat}_D^d \times D \) to be critical (Definition II.4): For \( X \in \text{Herm}_D = i \text{Lie}(K) \), we have that \( \partial_{t=0} \| e^{tX} \cdot M \|^2_2 \) is computed as

\[
\partial_{t=0} \sum_{i=1}^d \text{tr} \left[ (e^{tX} M(i)) e^{-tX} M(i)^\dagger e^{tX} M(i) e^{-tX} \right] \\
= \partial_{t=0} \sum_{i=1}^d \text{tr} \left[ (M(i)) e^{2tX} M(i) e^{-2tX} \right] \\
= 2 \text{tr} \left[ X \left( \sum_{i=1}^d (M(i)(M(i))^\dagger - (M(i))^\dagger M(i)) \right) \right] \quad (\text{III.5})
\]

Thus we arrive at the following (illustrated in Fig. 8):

**Theorem III.10 (Characterization).** Let \( M \in \text{Mat}_D^d \times D \). Then \( M \) is in minimal canonical form if and only if \( \| g \cdot M \|_2 \geq \| M \|_2 \) for all \( g \in \text{GL}(D) \). This is the case if and only if

\[
\sum_{i=1}^d M(i)(M(i))^\dagger = \sum_{i=1}^d (M(i))^\dagger M(i) \quad (\text{III.6})
\]

Equivalently, the reduced density matrices of \( \rho = |M\rangle \langle M| \) on the virtual bonds are the same up to a transpose:

\[
\rho_1 = \rho_2^T \quad (\text{III.7})
\]

**Proof.** Note that \( M \) is critical if and only if the derivative in Eq. (III.5) vanishes for all \( X \in \text{Herm}_D \). Thus both statements follow from Theorem II.5. \( \square \)

Given a tensor \( M \) it is perhaps at first glance surprising that there always exist gauge transformations \( g_k \in \text{GL}(D) \) such that \( \lim_{k \to \infty} g_k \cdot M \) satisfies the conditions in Eqs. (III.6) and (III.7) — yet as we just saw this follows readily from geometric invariant theory. We also note that Theorem III.10 also shows that the minimal canonical form for MPS will in general not coincide with the usual left or right canonical form (Definition III.5); there appears to be no obvious way to convert one into the other. In Section V we give a simple iterative algorithm that computes the minimal canonical form to arbitrary precision.

To get more intuition about the definition and the relevance of the orbit closure, we revisit Example III.4.

**Example III.11.** In Example III.4 we saw that the following matrix tuples \( M, \hat{M} \in \text{Mat}_2^2 \times 2 \) both define the GHZ states:

\[
M(0) = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \quad M(1) = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}
\]

and

\[
\hat{M}(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \hat{M}(1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}
\]

Theorem III.10 shows that \( \hat{M} \) is already in minimal canonical form, while \( M \) is not. Indeed, while \( \rho_1 = \rho_2^T = I_2 \) for \( \rho = |\hat{M}\rangle \langle \hat{M}| \), the reduced states of \( \rho = |M\rangle \langle M| \) satisfy

\[
\rho_1 = M(0)(M(0))^\dagger + M(1)(M(1))^\dagger = \begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix},
\rho_2^T = (M(0))^\dagger M(0) + (M(1))^\dagger M(1) = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.
\]

Moreover, in this example it is easy to see that there does not exist a \( g \in \text{GL}(2) \) such that \( g \cdot M \) is in minimal canonical form. However, if we let

\[
g_\varepsilon = \begin{pmatrix} \varepsilon & 0 \\ 0 & 1 \end{pmatrix}
\]

then we may verify that

\[
g_\varepsilon M(0) g_\varepsilon^{-1} = \begin{pmatrix} \varepsilon & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \varepsilon^{-1} & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & \varepsilon \\ 0 & 0 \end{pmatrix}
\]

\[
g_\varepsilon M(1) g_\varepsilon^{-1} = \begin{pmatrix} \varepsilon & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \varepsilon^{-1} & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & \varepsilon \\ 0 & 1 \end{pmatrix}
\]

so as we let \( \varepsilon \to 0 \) we see that \( g_\varepsilon \cdot M \to \hat{M} \), which as just discussed is in minimal canonical form.

**Example III.12.** An amusing special case is \( d = 1 \), so we have a single matrix \( M \in \text{Mat}_D^1 \times 1 \). The minimal canonical form is given by the diagonal matrix with the same eigenvalues as \( M \) (repeated according to their algebraic multiplicity). Indeed, there are matrices \( g_\varepsilon \) such that \( g_\varepsilon \cdot M = g_\varepsilon M g_\varepsilon^{-1} \) is in Jordan normal form, but with \( \varepsilon \) instead of 1 as the offdiagonal entries. Letting \( \varepsilon \to 0 \) we obtain the desired diagonal matrix.

From Examples III.11 and III.12 it is clear that, by virtue of considering the orbit closure, the minimal canonical form automatically sets off-diagonal blocks to zero, which is an additional step which needs to be manually taken in the usual approach to canonical forms for MPS (see Section III-A). There, as already commented in Section III-A, it may also be necessary to block together multiple sites. The geometric invariant theory approach makes these steps redundant.\(^6\)

We will now prove a fundamental theorem for MPS where this will become explicit. Before stating the result, we state the ingredient that will be used to prove it. In invariant theory, the action of the gauge group on MPS tensors (Definition III.2) is known as the simultaneous conjugation action of \( \text{GL}(D) \) on matrix tuples in \( \text{Mat}_D^d \times D \). There, it is known that the ring of invariant polynomials is generated precisely by the coefficients (III.1) of the corresponding matrix product states for system size \( 1 \leq n \leq D^2 \), as stated in the following theorem [73]–[76]:

\^[6]As a side remark, there is actually no need to block in the usual canonical form for MPS. This is a consequence of Theorem 16 in [72], together with the overlooked observation that the matrix \( Z \) appearing there can be absorbed in another gauge transformation.\]
Theorem III.13 (Procesi-Razmyslov-Formanek). The invariant ring for the simultaneous conjugation action, i.e., $\mathbb{C}[\text{Mat}^d_{D \times D}]^{\text{GL}(D)}$, is generated by the invariant polynomials $P_i$, where

$$P_i(M) = (i_1, \ldots, i_n | M_n) = \text{tr} M^{(i_1)} \cdots M^{(i_n)},$$

for all $i = (i_1, \ldots, i_n) \in [d]^n$ and $n \in \mathbb{N}$. Moreover, it suffices to restrict to $n \in [D^2]$.

Thus, geometric invariant theory implies that gauge equivalence of the tensors (which by Theorem III.9 is captured by the minimal canonical form) is precisely equivalent to equality of the corresponding matrix product states! We summarize this in the following fundamental theorem for MPS (note that it works in full generality, without the need to block sites or remove off-diagonal terms):

Theorem III.14 (Fundamental theorem for MPS). Let $M, N \in \text{Mat}^d_{D \times D}$. Then the following are equivalent:

1) $M$ and $N$ are gauge equivalent (Definition III.7), i.e., $\text{GL}(D) \cdot M \cap \text{GL}(D) \cdot N \neq \emptyset$.
2) $|M_n) = |N_n)$ for all $n \in \mathbb{N}$.
3) $|M_n) = |N_n)$ for $n = 1, \ldots, D^2$.

Proof. This follows from Theorems II.9 and III.13. □

Remark III.15. It is also known that the invariant ring is not generated when restricting to $n \leq D^2/8$ [75]. However, while a system of generators of the invariant ring always suffices to separate orbit closures, this is in fact not necessary. Theorem 1.14 in [60] shows that the third condition in Theorem III.14 can be improved almost quadratically to:

3’ $|M_n) = |N_n)$ for $n = 1, \ldots, 4D \log_2 D + 12D - 4$, and it has been conjectured that $n = O(D)$ suffices [77]. Example III.17 shows that this is essentially tight.

Example III.16. In Example III.4 we saw two matrix tuples $M, \hat{M} \in \text{Mat}^2_{2 \times 2}$ that defined the GHZ states, for all system sizes. By our fundamental theorem, Theorem III.14, this implies that they are gauge equivalent, meaning that $\text{GL}(D) \cdot M \cap \text{GL}(D) \cdot \hat{M} \neq \emptyset$.

Now, in Example III.11 we saw that $\hat{M}$ is already in minimal canonical form. By the Kempf–Ness theorem (Theorem II.5) this means that the orbit of $\hat{M}$ is already closed. It follows that $\hat{M} \in \text{GL}(D) \cdot M$, which is in exact agreement with what we saw in Example III.11.

Example III.17. We also revisit Example III.12, the case of a single matrix. For $M, N \in \text{Mat}_D$, the equality of quantum states means that $\text{tr} M^n = \text{tr} N^n$ for all $n$, which is the case if and only if $M, N$ have the same characteristic polynomial and hence the same eigenvalues – in agreement with the discussion in Example III.12. Thus we see that in this special case it suffices to have equality for all $n = 1, \ldots, D$. This is also necessary, since, e.g., for $M$ a $D \times D$-permutation matrix representing a $D$-cycle we have $\text{tr} M^n = 0$ for $1 \leq n < D$.

Together, Theorems III.9 and III.14 show that if $M, N$ are two matrix tuples in minimal canonical form that give rise to the same quantum states, then $M$ and $N$ are related by a unitary gauge symmetry. As a consequence, we can lift unitary symmetries to the virtual level. Again, we do not need to make any assumptions about the tensor $M$.

Corollary III.18 (Lifting symmetries). Suppose that $M, N \in \text{Mat}^d_{D \times D}$ are in minimal canonical form and $u \in \text{U}(d)$ is a unitary such that $u^\otimes n |M_n) = |N_n)$ for all $n \in \mathbb{N}$. Then there exists a unitary $U \in \text{U}(D)$ such that $(I \otimes I \otimes u) |M) = (U \otimes \hat{U} \otimes I) |N)$.

In other words, the action of $u$ on the physical degrees of $M$ is implemented by the gauge action of $U$ on $N$.

Proof. Let $M' \in \text{Mat}^d_{D \times D}$ be the matrix tuple defined by $|M') := (I \otimes I \otimes u) |M)$. Then $M'$ is also in minimal canonical form, since $u$ is unitary and hence we have $\|g \cdot M\| = \|g \cdot M'\|$ for all $g \in \text{GL}(D)$. Moreover, by construction it holds that $|M'_n) = u^\otimes n |M_n) = |N_n)$ for all $n \in \mathbb{N}$. Thus Theorem III.14 shows that $M'$ and $N$ are gauge equivalent, and it follows from Theorem III.9 that there exists a unitary gauge transformation $U \in \text{GL}(D)$ such that $U \cdot N = M'$.

We note that $U$ need not be unique; for instance, $M$ itself may have a stabilizer, i.e., there may exist $U \in \text{U}(D)$ such that $U \cdot M = M$. Indeed, this is exactly the case in which the MPS given by $M$ has a global on-site symmetry, for which Corollary III.18 reproduces, for the minimal canonical form, the known local characterization of symmetries on MPS [14] usually obtained via the left or right canonical form and Theorem III.6.

Such characterization is the key step in the classification of symmetry protected topological phases done in [11]–[13]. The connection is as follows. If a system is invariant under the action of an onsite (global) symmetry group $u_g$, one gets $u_g^\otimes n |\Psi_n) = |\Psi_n)$ for its ground state $|\Psi_n)$ (global phases do not play a relevant role here). Since $|\Psi_n)$ is known to be very well approximated by MPS one may want to solve equation $u_g^\otimes n |M_n) = |N_n)$ for the MPS generated by some tensor $M$. By Corollary III.18, this is characterized by the existence of $U_g \in \text{U}(D)$ such that $(I \otimes I \otimes u_g) |M) = (U_g \otimes \hat{U}_g \otimes I) |M)$. It is not difficult to see that $U_g$ must be a projective representation of the symmetry group. The classification of SPT phases is then given by all non-equivalent projective representations, which is precisely described by the second cohomology group of the group cohomology of the symmetry group. The general validity of this approach has been recently established by the groundbreaking results of Ogata [78].
The idea that the relevant topological content of a system lies in its boundary has also given rise to the study of a bulk-boundary correspondence, usually known in this context as “entanglement spectra” or “entanglement Hamiltonian” [79], in which one upgrades the boundary to a physical system and looks for a dictionary between bulk and boundary properties. This is precisely the reason that tensor networks have become rather popular in the context of AdS-CFT holography in quantum gravity. For this program it is rather crucial that the boundary representations of the physical on-site symmetries are indeed given themselves by unitary representations, which is precisely what Corollary III.18 guarantees for the MPS case.

Remark III.19. As commented in Section III-A, a MPS state can also be interpreted as a CP map on the virtual Hilbert spaces, where $M \in \text{Mat}^{d}_{D \times D}$ is interpreted such that the $M^{(i)}$ are Kraus operators of a CP map $\mathcal{E}$, usually called the transfer operator. Equivalently, the reduced state $\rho_{12}$ of the quantum state $\rho = |M\rangle\langle M|$ on both virtual Hilbert spaces is the Choi operator of $\mathcal{E}$. As explained above Definition III.5, the left and right canonical form conditions are equivalent to $\mathcal{E}$ either being completely positive trace-preserving (CPTP) or unital (CPU). This perspective is particularly useful when dealing with contractions of large or infinite uniform MPS (the thermodynamic limit).

What is the interpretation of the minimal canonical form in this perspective? It is not hard to see that a mixed quantum state $\rho_{12}$ with conjugate marginals (i.e., $\rho_1 = \rho_2^T$) that are full-rank contains exactly the same data as a CPTP map $\Phi$ along with a full-rank invariant density operator $\Omega$ (i.e., $\Phi(\Omega) = \Omega$). The isomorphism $\rho_{12} \mapsto (\Phi, \Omega)$ is defined by defining $\Phi = \Phi_{1 \rightarrow 2}$ as the CPTP map with Choi operator $\rho_{12}^{-1/2} \rho_{12}^{1/2}$ and $\Omega = \rho_2 = \rho_1^T$. If the marginals do not have full rank we can restrict to its support. By duality, this is in turn the same as a CP unital map $\phi$ along with a faithful invariant state $\omega$ in the algebraic sense: We have an isomorphism $(\Phi, \Omega) \mapsto (\phi, \omega)$, defined by taking $\phi = \Phi^{1\dagger}$ and $\omega(X) = tr(\Omega X)$. At this point we do not see a natural interpretation of these conditions for MPS contractions in the thermodynamic limit.

C. Canonical forms for MPS with open boundary conditions

We will now consider open boundary conditions. We use the invariant theory framework to define canonical forms, which in this case are closely related to well-known canonical forms. Then it is natural to fix the system size $n$, and to consider the non-uniform setting. Let

$$V = \bigoplus_{k=0}^{n-1} \text{Mat}^{d}_{D_k \times D_{k+1}}$$

where $D_0 = D_n = 1$. As usual, $d$ is the physical dimension and the $D_k$ are the bond dimensions (which may vary per bond). Let $M = (M_0, \ldots, M_{n-1}) \in V$, then the associated MPS state $|M\rangle$ (note that now we have a fixed system size) is defined by

$$\langle i_0 \ldots i_{n-1}|M\rangle = M_0^{(i_0)} M_1^{(i_1)} \cdots M_{n-1}^{(i_{n-1})}.$$

We let $G = GL(D_1) \times \cdots \times GL(D_{n-1})$ act on $V$ by gauge transformations. To define this action, let $g = (g_1, \ldots, g_{n-1}) \in G$ and $M = (M_0, \ldots, M_{n-1}) \in V$. Then the action is given by

$$g \cdot M = ((g_1)_1 \cdot M_0, (g_1)_2 \cdot M_1, \ldots, (g_{n-1})_{n-2} \cdot M_{n-2}, (g_{n-1})_1 \cdot M_{n-1}),$$

where for $M_i = (M_i^{(j)})_{j=1}^d$ we have

$$(g_i, g_{i+1}) \cdot M_i := (g_i M_i^{(j)} g_{i+1}^{-1})_{j=1}^d.$$

It is clear that the resulting MPS state is invariant under the action of $G$. For every ‘bond cut’ $k \in \{1, \ldots, n-1\}$, we let $W_k := \text{Mat}^{d_k \times D_k} \oplus \text{Mat}^{D_k \times d_{n-k}}$ and we define a $G$-action on $W_k$ by

$$g \cdot (w_{\text{left}}, w_{\text{right}}) = (gw_{\text{left}} g^{-1}, g w_{\text{right}}).$$

Then we have a map $\iota_k : V \rightarrow W_k$, which maps the vector of MPS tensors $M$ to a pair of ‘half-chain contractions’ $(M_{k, \text{left}}, M_{k, \text{right}})$

$$\langle i_0 \ldots i_{k-1}|M_{k, \text{left}} = M_0^{(i_0)} M_1^{(i_1)} \cdots M_{k-1}^{(i_{k-1})}$$

$$M_{k, \text{right}} |i_k \ldots i_{n-1} = M_{k-1}^{(i_{k-1})} M_{k}^{(i_k)} \cdots M_{n-1}.$$  

This map is clearly $G$-equivariant. We can patch the maps $\iota_k$ together to obtain a $G$-equivariant polynomial map

$$\iota : V \rightarrow W := \bigoplus_{k=1}^{n-1} W_k.$$

We can think of $M_{k, \text{left}}$ and $M_{k, \text{right}}$ as the states where we have contracted all the bonds except the $k$-th. In this perspective the reduced density matrices on the left and right copies of $C^{D_k}$ are given by

$$\rho_{k, \text{left}} = \sum_i (M_i^{(k-1)})^\dagger \cdots (M_0^{(i_0)})^\dagger M_{k-1}^{(i_k-1)}$$

$$= M_{k, \text{left}}^\dagger M_{k, \text{left}}$$

and

$$\rho_{k, \text{right}} = \sum_i M_{k-1}^{(i_k)} \cdots M_{n-1}^{(i_{n-1})} (M_{n-1}^{(i_{n-1})})^\dagger \cdots (M_k^{(i_k)})^\dagger$$

$$= M_{k, \text{right}} M_{k, \text{right}}^\dagger.$$

We claim that norm minimization in the image of $\iota$ leads to a canonical form where $\rho_{k, \text{left}} = \rho_{k, \text{right}}^\dagger$, which we call the minimal canonical form for non-uniform MPS:

Definition III.20. Let $M \in V$. Then $M_{\text{min}}$ is a minimal canonical form for $M$ if $\iota(M_{\text{min}})$ is an element of minimal norm with respect to the orbit closure $G \cdot M$, i.e.,

$$M_{\text{min}} = \arg \min \{\|\iota(M')\|_2 : M' \in GL(D) \cdot M\}.$$

The norm we are considering here is again the Euclidean one. Note also that $g \cdot \iota_k(M)$ only depends on $g_k$. Therefore, we may also write $g_k \cdot \iota_k(M)$. In minimizing $\|g \cdot \iota(M)\|_2$ we may minimize each $\|g_k \cdot \iota_k(M)\|_2$ separately. By the same
general theory as applied in Section III-B we deduce that the canonical form exists and is unique up to conjugation by unitary elements in \( G \). Moreover, as in Theorem III.10 we may set an appropriate derivative equal to zero to find a condition for when \( M \) is in minimal canonical form.

Letting \( g_k(t) = e^{\lambda X_k} \) for \( X_k \in \text{Her}
(\lambda) \), we see that
\[
\|g_k(t) \cdot \varepsilon_k(M)\|_2^2 = \text{tr}[g_k(t)^{-1} M_{k,\text{left}}^\dagger M_{k,\text{left}} g_k(t)^{-1}]
\]

\[
+ \text{tr}[e^{-2 \lambda X_k} M_{k,\text{right}}^\dagger M_{k,\text{right}} g_k(t)]
\]

and hence, denoting by \( g(t) = (g_1(t), \ldots, g_{n-1}(t)) \) we have that \( \partial_{t=0} \|g(t) \cdot M\|_2^2 \) is given by
\[
\partial_{t=0} \sum_{k=1}^{n-1} \|g_k(t) \cdot \varepsilon_k(M)\|_2^2 = 2 \sum_{k=1}^{n-1} \text{tr} \left[ X_k \left( M_{k,\text{right}} M_{k,\text{left}}^\dagger - M_{k,\text{right}}^\dagger M_{k,\text{left}} \right) \right].
\]

Setting this equal to zero is equivalent to \( \rho_{k,\text{left}} = \rho_{k,\text{right}}^T \) for all \( k \).

We may explicitly perform the minimization; it is closely related to Vidal’s canonical form [80]. We can perform a singular value decomposition
\[
M_{k,\text{left}} = V_1 \Sigma_1 U_1
\]
where \( V_1 \in \text{Mat}_{d^k \times D_k} \) is an isometry, \( \Sigma_1 \in \text{Mat}_{D_k \times D_k} \) is diagonal with nonnegative entries and \( U_1 \in \text{Mat}_{D_k \times D_k} \) is unitary. Next, we perform a singular value decomposition on \( \Sigma_1 U_1 M_{k,\text{right}} \) so
\[
\Sigma_1 U_1 M_{k,\text{right}} = U_2 \Sigma_2 V_2
\]
where \( V_2 \in \text{Mat}_{D_k \times D_k} \) is an isometry, \( \Sigma_2 \in \text{Mat}_{D_k \times D_k} \) is diagonal with nonnegative entries and \( U_2 \in \text{Mat}_{D_k \times D_k} \) is unitary. Let \( \Pi_1 \) be the projection onto \( \text{ker}(\Sigma_1) \) and let \( \Sigma_1 = \Sigma_1 + \Pi_1 \). Then let
\[
g_k = \sqrt{\Sigma_2^{-1} U_2^\dagger \Sigma_1 U_1}
\]
and we let \( \tilde{M}_{k,\text{left}} = M_{k,\text{left}}^\dagger g_k^{-1} \) and \( \tilde{M}_{k,\text{right}} = g_k M_{k,\text{right}} \). Then we may verify that the associated reduced density matrices are
\[
\rho_{k,\text{left}} = \tilde{M}_{k,\text{left}}^\dagger \tilde{M}_{k,\text{left}} = \sqrt{\Sigma_2^{-1} U_2^\dagger \Sigma_1 U_1 M_{k,\text{left}}^\dagger M_{k,\text{left}}} \Sigma_1^{-1} U_2 \sqrt{\Sigma_2} = \Sigma_2
\]
and
\[
\rho_{k,\text{right}}^T = \tilde{M}_{k,\text{right}} \tilde{M}_{k,\text{right}}^\dagger = \sqrt{\Sigma_2^{-1} U_2^\dagger \Sigma_1 U_1 M_{k,\text{right}} M_{k,\text{right}}^\dagger U_1^\dagger \Sigma_1 U_2 \sqrt{\Sigma_2}^{-1} = \Sigma_2.
\]

Therefore, defining \( g_k \) in this fashion for each \( k \) gives \( g \cdot M \) in minimal canonical form. In this case it is not necessary to go to the closure to obtain the canonical form.

This canonical form coincides with the one of Vidal [80], usually written in the form
\[
\sum_{i_0, \ldots, i_{n-1}} \Gamma^{(i_0)}_{0} \Lambda^{(i_1)}_{1} \Lambda^{(i_2)}_{2} \cdots \Lambda^{(i_{n-1})}_{n-1} |i_0, i_{n-1}\rangle \langle i_0, i_{n-1}| \quad (III.8)
\]
if one identifies \( \Lambda^{(i_k)}_{k} \) with \( \sqrt{\Lambda^{(i_k)}_{k}^\dagger} \sqrt{\Lambda^{(i_{k+1})}_{k+1}} \). The reason is that, by the properties of Vidal’s canonical form [80], [81], such choice fulfills the algebraic characterization of the minimal canonical form given by \( \rho_{k,\text{left}} = \rho_{k,\text{right}}^T \) for all \( k \).

Since the positive diagonal matrices \( \Lambda_k \) correspond to the Schmidt coefficients of the bipartition of the system in the cut \( [0 : k-1], [k-1] \), the minimal canonical form can be understood in this case as an even distribution of those weights. This particular distribution of weights has also appeared extensively in the standard MPS literature [82].

There are also left and right canonical forms [81]. These fit in the same framework, which we will now show for the left canonical form (with the right canonical form being completely analogous). Let \( V \) be as before, but now we consider the action of \( G = \text{SL}(D_1) \times \cdots \times \text{SL}(D_{n-1}) \). We let \( W_k = \text{Mat}_{d^k \times D_k} \) (which is only the left half chain) and we let \( \varepsilon_k : V \to W_k \) be given by \( M_k = \varepsilon_k(M) \)
\[
| i_0 \cdots i_{k-1} \rangle M_k = M_0^{(i_0)} M_1^{(i_1)} \cdots M_{k-1}^{(i_{k-1})}
\]
(so this is what previously was \( M_{k,\text{left}} \)). The group action is given by the \( M_k \to M_k g_k^{-1} \). We similarly define
\[
\iota : V \to W := \bigoplus_{k=1}^{n-1} W_k.
\]

Computing the gradient as before, but now restricting to traceless \( X \) (as we are optimizing over \( \text{SL}(D_k) \)) we find that at the minimum of the norm \( \|g \cdot M\|_2 \) the reduced density matrix \( \rho_{k,\text{left}} \) must be proportional to the identity for all \( k \). Again, we can explicitly realize the minimum, without going to the closure. To this end we perform a singular value decomposition \( M_k = V \Sigma_k U \). Let \( \Pi_2 \) be the projection onto \( \text{ker}(\Sigma_2) \) and let \( \Sigma_2 = \Sigma_2 + \Pi_2 \). Then taking
\[
g_k = \det(\Sigma U)^{-1/2} \Sigma U \in \text{SL}(D_k)
\]
yields a uniform reduced density matrix \( \rho_{k,\text{left}} \).

IV. PROJECTED ENTFLED PAIR STATES

In this section we start by defining projected entangled pair states (PEPS), in particular uniform PEPS. In Section IV-B we introduce the minimal canonical form for PEPS. We will see that by closely analogous arguments to the MPS case we may establish its basic properties. In Section IV-D we relate to two-dimensional tilings and explain how our results are compatible with earlier no-go results for the existence of canonical forms for PEPS. In Section IV-E we study in more detail the role of the orbit closure and show that in many cases of interest the orbit is closed.
A. Definition of uniform PEPS

We will now define a generalization of MPS, known as Projected Entangled Pair States (PEPS). We start by defining a rather general version, and then specialize to cases of interest. As input we require a graph $\Gamma = (V, E)$ and dimensions $(d_v)_{v \in V}$ (the bond dimensions) and $(d_e)_{e \in V}$ (the physical dimensions). Let $E(v)$ denote the set of edges incident to $v \in V$. Then we let $\mathcal{H}_v := \mathbb{C}^{d_v}$, and for each $e \in E(v)$ we let $\mathcal{H}_{v,e} := \mathbb{C}^{d_e}$. The PEPS will now be constructed from a collection of tensors $(T^v)_v \in \mathcal{H}_{v,e}$ where

$$T^v \in \bigotimes_{e \in E(v)} \mathcal{H}_{v,e} \otimes \mathcal{H}_v.$$

The resulting PEPS is a state on $\bigotimes_{v \in V} \mathcal{H}_v$, and is constructed by ‘contracting along the edges’. If $e = (v, w)$ is an edge incident to $v$ and $w$, then the contraction map $\delta_e : \mathcal{H}_{v,e} \otimes \mathcal{H}_{w,e} \to \mathcal{H}_e$ along $e$ is defined by

$$|ij\rangle \mapsto \delta_{i,j}$$

and extending by linearity. We may apply these maps along each of the edges in $E$ and this yields a state $|T\rangle$ on $\bigotimes_{v \in V} \mathcal{H}_v$.

A clean way of writing this contraction operation (and also explaining the nomenclature projected entangled pair states) is by the identity

$$|T\rangle = \left( \bigotimes_{e \in E(v)} \left( \sum_{i=0}^{D_e-1} (ii) \right) \otimes I_V \right)_{v \in V} \prod_{v \in V} T^v,$$

where $I_V$ is the identity operator on $\bigotimes_{v \in V} \mathcal{H}_v$.

We will now specialize to the case of uniform PEPS. In this case we place the same tensor at each vertex. It is natural to contract the tensors placed on periodic grids in $m$ spatial dimensions, but we will see that other graphs are also relevant. We denote the physical dimension by $d$ and the associated physical Hilbert space by $\mathcal{H}_{\text{phys}} = \mathbb{C}^d$, and there are $m$ relevant bond dimensions in the different directions, which we will denote by $D_k$ for $k \in [m]$. For each direction $k \in [m]$ we have two Hilbert spaces $\mathcal{H}_{k,1} = \mathbb{C}^{D_k}$ and $\mathcal{H}_{k,2} = \mathbb{C}^{D_k}$. Similar to the MPS case, we may interpret the PEPS tensor $T$ either as a tensor

$$|T\rangle \in \bigotimes_{k=1}^m \mathcal{H}_{k,1} \otimes \mathcal{H}_{k,2} \otimes \mathcal{H}_{\text{phys}}$$

or as a matrix tuple

$$T = (T^{(i)})_{i=1}^d, \quad T^{(i)} \in \bigotimes_{j=1}^m \text{Mat}_{D_j \times D_j}$$

and we will generally identify this space of matrix tuples as $\text{Mat}_{D_1 \times D_m}$. Typically, one constructs corresponding quantum states by placing copies of the tensor on a grid and contracting along the bond dimensions, see Fig. 9.

Definition IV.1 (Uniform PEPS on a grid). For any matrix tuple $T = (T^{(i)})_{i=1}^d \in \text{Mat}_{D_1 \times D_m}^{D_1 \times D_m}$ and system sizes $n_1, \ldots, n_m \in \mathbb{N}$, we define the uniform (or translation-invariant) projected entangled pair state (PEPS) as the (not necessarily) quantum state $|T_{n_1, \ldots, n_m}\rangle \in (\mathbb{C}^d)^\otimes n$, where $n := n_1 \cdots n_m$ and which is given by contracting $n$ copies of $T$ on an $n_1 \times \cdots \times n_m$ periodic grid.

We would like to allow a broader class of uniform PEPS, where one may use in principle any possible contraction graph. In such a contraction graph we only demand that the directions are matched up, in the sense that we always contract $\mathcal{H}_{k,1}$ with $\mathcal{H}_{k,2}$. A natural way to express such contractions is as follows. Suppose that we have $n$ vertices, with at each vertex a copy of $T$, and we are given a contraction graph. We will define permutations $\pi_k \in S_n$ for each direction $k \in [m]$. Suppose that in direction $k$ $\alpha, \beta \in [n]$ are such that the Hilbert space $\mathcal{H}_{k,1}$ of the $\alpha$-th copy of $T$ is contracted with the Hilbert space $\mathcal{H}_{k,2}$ of the $\beta$-th copy of $T$, then we let $\pi_k$ map $\alpha$ to $\beta$. Each contraction map (and ordering of the vertices) then uniquely determines permutations $\pi_k \in S_n$. As permutations $\pi = (\pi_1, \ldots, \pi_m)$ completely determine the contraction of the $n$ copies of $T$ to a quantum state on $\mathcal{H}_{\text{phys}}^\otimes n = (\mathbb{C}^d)^\otimes n$ we denote this state by $|T_{\pi}\rangle$. For $k \in [m]$ let $R_{\pi_k}$ be the operator on $(\mathbb{C}^{D_k})^\otimes n$ permuting the $n$ tensor factors.

Definition IV.2 (Uniform PEPS on arbitrary contraction graphs). For any tensor $T = (T^{(i)})_{i=1}^d \in \text{Mat}_{D_1 \times D_m}^{D_1 \times D_m}$, system size $n$ and for $\pi = (\pi_1, \ldots, \pi_m) \in S_n$ we define the associated uniform projected entangled pair state (PEPS) as the (not necessarily) quantum state $|T_{\pi}\rangle \in (\mathbb{C}^d)^\otimes n$ which has coefficients defined by

$$\langle i_1, \ldots, i_n | T_{\pi}\rangle = \text{tr} \left[ R_{\pi_1} \otimes \cdots \otimes R_{\pi_m} T^{(i_1)} \otimes \cdots \otimes T^{(i_n)} \right]$$

for $i = (i_1, \ldots, i_n) \in [d]^n$.

We may use the coefficients of the contracted state $|T_{\pi}\rangle$ to define functions $P_{\pi, i} \in \mathbb{C}[\text{Mat}_{D_1 \times D_m}^{D_1 \times D_m}]$ as

$$P_{\pi, i}(T) = \langle i_1, \ldots, i_n | T_{\pi}\rangle.$$  \hfill (IV.3)

For $m = 1$ we get back the usual notion of MPS. Note that in this case, if we assume the contraction graph to be connected, there is a unique way to contract the tensors, corresponding to any full cycle in $S_n$. Indeed, for $T \in \text{Mat}_{D \times D}$ and $\pi = (1 \ldots n) \in S_n$ we see that $|T_{\pi}\rangle = |T_n\rangle$ as defined in Eq. (III.1).

We also note that we recover the notion of uniform PEPS on a grid by choosing appropriate permutations. For instance, for $m = 2$, and a grid of size $n_1 \times n_2$ this would correspond to using the permutations

$$\pi_1 = (1 \ldots n_1)(n_1 + 1 \ldots 2 n_1) \ldots$$

$$\ldots ((n_2 - 1)n_1 + 1 (n_2 - 1)n_1 + 2 \ldots n_2 n_1)$$

$$\pi_2 = (1 n_1 + 1 \ldots (n_2 - 1)n_1 + 1) (2 n_1 + 2 \ldots$$

$$\ldots (n_2 - 1)n_1 + 2) (n_1 2 n_1 \ldots n_2 n_1).$$

This yields (upon appropriately identifying the copies of $\mathcal{H}_{\text{phys}}$) an equivalence $|T_{n_1, n_2}\rangle = |T_{\pi_1, \pi_2}\rangle$. 

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As in the MPS case, we have a ‘gauge group’ acting on the tensor. We can now act with a different group element along each direction \( k \in [m] \).

**Definition IV.3** (Gauge action). We define the gauge action of \( g \in G = \text{GL}(D_1) \times \cdots \times \text{GL}(D_m) \), where \( g = (g_1, \ldots, g_m) \), on \( T \in \text{Mat}^{d_1 \times \cdots \times d_m}_{D_1 \times \cdots \times D_m} \) as

\[
g \cdot T = \left( (g_1 \otimes \cdots \otimes g_m) T^{(i)} (g_1^{-1} \otimes \cdots \otimes g_m^{-1}) \right)_{i=1}^d.
\]

If we think of \( T \) as a quantum state \( |T\rangle \) in the Hilbert space \( (\bigotimes_{i=1}^m \mathcal{H}_{k,i} \otimes \mathcal{H}_{k,2}) \otimes \mathcal{H}_{\text{phys}} \), the gauge action can be written as

\[
g \cdot |T\rangle = \left( \left( \bigotimes_{k=1}^m g_k \otimes g_k^T \right) \otimes I \right) |T\rangle.
\]

As in the MPS case, it is easy to see that this action keeps the associated PEPS invariant. By continuity, this is also true after taking limits, giving rise to the following lemma.

**Lemma IV.4.** For every \( T \in \text{Mat}^{d_1 \times \cdots \times d_m}_{D_1 \times \cdots \times D_m} \) and for \( G = \text{GL}(D_1) \times \cdots \times \text{GL}(D_m) \), if \( T^\pi \in G \cdot T \), then for all \( \pi \in S_m^m \)

\[
|T^\pi\rangle = |T^\pi\rangle.
\]

and in particular

\[
P_{\pi,k}(T) = P_{\pi,k}(T').
\]

In other words, the coefficient functions \( P_{\pi,k} \) are polynomials in the invariant ring \( \mathbb{C}[\text{Mat}^{d_1 \times \cdots \times d_m}_{D_1 \times \cdots \times D_m} T] \). We have a corresponding notion of gauge equivalence.

**Definition IV.5** (Gauge equivalence). Let \( S \) and \( T \) be tensors \( S, T \in \text{Mat}^{d_1 \times \cdots \times d_m}_{D_1 \times \cdots \times D_m} \). Let \( G \) be the group \( \text{GL}(D_1) \times \cdots \times \text{GL}(D_m) \). We say that \( S \) and \( T \) are gauge equivalent if and only if

\[
G \cdot S \cap G \cdot T \neq \emptyset.
\]

**B. Minimal canonical form**

We consider uniform PEPS in \( m \) spatial dimensions with bond dimensions \( D_1, \ldots, D_m \) and physical dimension \( d \). We denote the gauge group by \( G = \text{GL}(D_1) \times \cdots \times \text{GL}(D_m) \). We denote by \( K = U(D_1) \times \cdots \times U(D_m) \subset G \) the unitary subgroup. We can now follow exactly the same approach as in the MPS case to define the minimal canonical form, and the same general results from geometric invariant theory allow us to prove its basic properties.

**Definition IV.6** (Minimal canonical form PEPS). We say \( T_{\min} \in \text{Mat}^{d_1 \times \cdots \times d_m}_{D_1 \times \cdots \times D_m} \) is a minimal canonical form of \( T \in \text{Mat}^{d_1 \times \cdots \times d_m}_{D_1 \times \cdots \times D_m} \) if it is an element of minimal norm in the orbit closure \( G \cdot T \), i.e.,

\[
T_{\min} = \text{arg min} \{ \|S\|_2 : S \in G \cdot T \}.
\]

We say \( T \in \text{Mat}^{d_1 \times \cdots \times d_m}_{D_1 \times \cdots \times D_m} \) is in canonical form if it is a minimal canonical form for itself, i.e. an element of minimal norm in \( G \cdot T \).

The norm considered in the definition is, as in the MPS case, the Euclidean norm of \( T \) (or \( |T\rangle \)):

\[
\|T\|_2 = \sqrt{\langle T | T \rangle} = \left( \sum_{i=1}^d \text{tr} \left( (T^{(i)})^\dagger T^{(i)} \right) \right)^{1/2}.
\]

The minimal canonical form is not uniquely defined, but it is unique up to the action by the unitary group \( K = U(D_1) \times \cdots \times U(D_m) \):

**Theorem IV.7** (Minimal canonical form). Let \( S \) and \( T \) be tensors \( S, T \in \text{Mat}^{d_1 \times \cdots \times d_m}_{D_1 \times \cdots \times D_m} \). Then the following are equivalent:

1. \( S \) and \( T \) have a common minimal canonical form.
2. If \( S_{\min} \) and \( T_{\min} \) are minimal canonical forms for \( S \) and \( T \), then \( K \cdot S_{\min} = K \cdot T_{\min} \).
3. \( S \) and \( T \) are gauge equivalent, i.e., \( G \cdot S \cap G \cdot T \neq \emptyset \).

**Proof.** This is an immediate consequence of Theorem II.3. \( \Box \)

Recall that if \( T \in \text{Mat}^{d_1 \times \cdots \times d_m}_{D_1 \times \cdots \times D_m} \) is a PEPS tensor, we saw in Eq. (IV.1) that we may consider it as a quantum state \( |T\rangle \). For each ‘direction’ \( k \in [m] \), we have two virtual Hilbert spaces \( \mathcal{H}_{k,1} \) and \( \mathcal{H}_{k,2} \) of dimension \( D_k \) and there is the physical Hilbert space \( \mathcal{H}_{\text{phys}} \) of dimension \( d \). We denote by \( \rho_{k,j} \) the reduced state of \( \rho = |T\rangle \langle T| \) on \( \mathcal{H}_{k,j} \).

The characterization of minimum norm vectors as critical norm vectors in Theorem II.5 can be used to give a condition for a tensor to be in minimal canonical form. To find this condition we perform a computation similar to the MPS case. We identify \( i \text{Lie}(K) \) with \( \text{Herm}_{D_1} \times \cdots \times \text{Herm}_{D_m} \) and compute for \( X = (X_1, \ldots, X_m) \in \text{Herm}_{D_1} \times \cdots \times \text{Herm}_{D_m} \). If we write

\[
\hat{X}_k = I_{D_1} \otimes \cdots \otimes X_k \otimes \cdots \otimes I_{D_m}
\]

and

\[
e^{i t} X = e^{2i t X_1} \otimes \cdots \otimes e^{2i t X_m},
\]
Theorems. For MPS we already saw such fundamental theorems, Theorem IV.8. The tensor \( T \) is injective if it is injective as a map from the virtual legs to the extended to the general case in [31].

Proof. By Theorem II.5, \( T \) is in minimal canonical form if and only if \( \| g \cdot T \|_2 \geq \| T \|_2 \) for all \( g \in G \). This is the case if and only if the reduced density matrices of \( \rho = [T] \) on the virtual bonds are the same in each direction, up to a transpose:

\[
\rho_{k,1} = \rho_{k,2}^T \quad (\forall k \in [m]) \quad (IV.5)
\]

These conditions are illustrated in Fig. 10 for \( m = 2 \). Without the framework of invariant theory, it is not clear that one can indeed transform any tensor by gauge transformations to satisfy the conditions in Theorem IV.8. This is an important difference with earlier proposals for canonical forms for PEPS. For instance, [35] proposes a canonical form based on a similar (but different) condition. However, in that case, it is not clear that such a canonical form indeed exists for any tensor.

Both Theorem IV.7 and Theorem IV.8, giving the “uniqueness” of the canonical form and its algebraic characterization respectively, only require situations in which one is already interested in analyzing tensors related by gauge transformations. Reducing to such a situation is the goal of the Fundamental Theorems. For MPS we already saw such fundamental theorems, in particular Theorem III.14, which apply to general MPS.

For PEPS the situation is more complicated, but for important special cases, fundamental theorems are known. In particular, fundamental theorems are known for the family of normal tensors [64], proven for the uniform 2D case in [83], and extended to the general case in [31].

To define normal tensors, we first recall the notion of an injective PEPS tensor. A tensor \( T \in \text{Mat}_{d_1 \ldots d_m}^{D_1 \ldots D_2} \) is injective if it is injective as a map from the virtual legs to the physical legs, i.e. if it is injective as a \( d \times D_1^2 \ldots D_2^m \) matrix. The tensor \( T \) is normal if it is injective after blocking together a number of copies to a single new tensor. Let us explain what we mean by ‘blocking’. Given \( T \in \text{Mat}_{d_1 \ldots d_m}^{D_1 \ldots D_2} \), we can contract \( n \) copies of \( T \) on a rectangular lattice of size \( n_1 \times \cdots \times n_m \) sites to obtain a new tensor \( \tilde{T} \) with physical dimension \( d^n \) and bond dimensions \( D_1^{n_2} \ldots D_2^{n_m} \). The tensor \( T \) is normal if there exists some blocking such that the resulting tensor \( \tilde{T} \) is injective.

Hence in the normal case, which is a generic condition, Theorem IV.7 and Theorem IV.8 together with the Fundamental Theorem of [83] already apply to show the following statement (for simplicity we only write down the two-dimensional case):

**Corollary IV.9.** If we are given normal tensors \( T \) and \( S \) in \( \text{Mat}_{D_1, D_2}^{D_1, D_2} \), then they define the same state in all \( n_1 \times n_2 \) grids, i.e. \( [T_{n_1, n_2}] = [S_{n_1, n_2}] \) for all \( n_1, n_2 \in \mathbb{N} \), if and only if their corresponding minimal canonical forms \( S_{\text{min}} \) and \( T_{\text{min}} \) are related by local unitary gauges: \( S_{\text{min}} = U \cdot T_{\text{min}} \) for a suitable unitary \( U \in \text{U}(D_1) \times \text{U}(D_2) \).

Moreover, we will see below in Proposition IV.20 that the orbit of a normal tensor is always closed. However, this is not the end of the story. There are other (non-normal) tensors which define the same state in all \( n_1 \times n_2 \) grids, but are nevertheless not related by a gauge transformation. An explicit example appears in [84], in the context of 2D SPT phases. We provide the example here:

**Example IV.10.** The idea of the example is simple but ingenious. Take pairs of MPS normal tensors \( A \) and \( B \) so that \( |A_i⟩ = |B_i⟩ \) but \( |A_j⟩ \neq |B_j⟩ \) for all \( j > 4 \).\(^7\) The explicit examples of [84] have physical dimension 2 and are given by the matrices:

\[
A^{(1)} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad A^{(2)} = \begin{pmatrix} 24 & -10 \\ 17 & -3 \end{pmatrix},
\]

where \( B^{(1)} = A^{(1)} \) and \( B^{(2)} = -A^{(2)} \).

Now, in each vertex of a two dimensional grid, place four qubits and, by joining each one of those qubits with the closest one in each of the nearest neighbor sites, fill in the lattice with a set of non-overlapping plaquettes \( P \). The states we are interested are \( |M_A⟩ = \bigotimes_{p \in P} |A_p⟩ \) and \( |M_B⟩ = \bigotimes_{p \in P} |B_p⟩ \). It is now obvious how to define the associated PEPS tensors \( M_A \) and \( M_B \) for the vertices. Just take, with the appropriate identification of indices, \( M_A = A^{(1)} \otimes A^{(2)} \) and \( M_B = B^{(1)} \otimes B^{(2)} \) (recall that each vertex contains four qubits and therefore the physical dimension is 16). It is shown in [84] that tensors \( M_A, M_B \) are not in the same \( \text{GL}_4 \times \text{GL}_4 \) orbit. One can indeed show that the closure of their orbits do not intersect. One possibility is just to realize that, because of the symmetry of the tensors \( M_A \) and \( M_B \), they are already in minimal canonical form, and therefore their orbits are already closed. The other possibility is to compare \( M_A \) and \( M_B \) in different contraction graphs \( \Gamma \).

\(^7\)It is only proven in [84] that \( |A_5⟩ \neq |B_5⟩ \), but since it is also shown that both \( A \) and \( B \) become injective when blocking two sites, known bounds for the fundamental theorem [31] imply already that if \( |A_i⟩ = |B_i⟩ \) for any \( j \geq 6 \), then \( A \) and \( B \) would be gauge-related and then \( |A_5⟩ = |B_5⟩ \).
It is easy to find some $\Gamma$ for which the length of some of the plaquettes are larger than 4 and then the fact that $|A_j| \neq |B_j|$ for $j > 4$ implies that the associated states $|M_{A,\Gamma}|$ and $|M_{B,\Gamma}|$ are different, which in turn implies that the orbits of $M_A$ and $M_B$ cannot intersect.

C. Fundamental theorem and invariant theory of uniform PEPS

This example makes clear that we have to change perspective to derive a Fundamental Theorem which is an analog to the MPS one (Theorem III.14). Instead of starting with the condition $|S_{n_1,n_2}| = |T_{n_1,n_2}|$ for all $n_1, n_2$, and asking how the tensors $S$ and $T$ are related, we start with the condition that $S$ and $T$ are gauge equivalent, and we ask how we can characterize this based on the corresponding tensor network states. It turns out that we need to compare the states not just on grids, but on arbitrary contraction graphs. That is, the appropriate conditions is $|S_{\pi}| = |T_{\pi}|$ for tuples of permutations $\pi$.

Additionally, for MPS we found that it suffices to consider systems of size at most $D^2$ (Theorem III.14) or even $O(D)$ (Remark III.15). For $m \geq 2$ we prove a similar bound, but now we need a system size exponential in $D$ (and we show below, in Proposition IV.15, that this exponential dependence cannot be avoided). Formally, we have the following weak version of a Fundamental Theorem, illustrated in Fig. 5.

**Theorem IV.11** (Fundamental Theorem for PEPS). Let $S, T$ be tensors in $\text{Mat}^d_{D_1...D_m \times D_1...D_m}$. Then the following are equivalent:

1. The $G$-orbit closures of $S$ and $T$ intersect, i.e., $\overline{G \cdot S \cap G \cdot T} \neq \emptyset$.
2. $|S_{\pi_1,...,\pi_m}| = |T_{\pi_1,...,\pi_m}|$ for all $\pi_k \in S_r$ for all $r \in \mathbb{N}$.
3. $|S_{\pi_1,...,\pi_m}| = |T_{\pi_1,...,\pi_m}|$ for all $\pi_k \in S_r$ for $r \leq \exp(cnD^2\log D)$ where $D = \max\{D_1,...,D_m\}$ and $c$ is a constant.

To prove this result, we start with the fundamental result in invariant theory [85, §4.6], which allows us to deduce the study of invariant polynomials over homogeneous degree $n$ in the ring of invariant polynomials $\mathbb{C}[\text{Mat}^d_{D \times D}]^G$ to the study of multilinear invariant polynomials. While the result is a basic one, it is a key component in proving a number of fundamental theorems in invariant theory, see [85] for more details.

**Lemma IV.12.** For any subgroup $G \subseteq GL(D)$, any polynomial $P$ in the ring of invariant polynomials $\mathbb{C}[\text{Mat}^d_{D \times D}]^G$ can be written as a linear combination of multihomogeneous invariant polynomials $P_n$ of some multidegree $n = (n_1, \ldots, n_d)$, each of which can be written as

$$P_n(M^{(1)}, \ldots, M^{(d)}) = Q(M^{(1)}, \ldots, M^{(1)}, \ldots, M^{(d)}, \ldots, M^{(d)}),$$

where $Q$ is a multilinear $G$-invariant polynomial in $n = \sum_{i=1}^d n_i$ matrix variables.

**Proof.** Let $P = P(M^{(1)}, \ldots, M^{(d)}) \in \mathbb{C}[\text{Mat}^d_{D \times D}]^G$. First we show that we may assume that $P$ is multihomogeneous, i.e., homogeneous of some degree $n_i$ in each matrix variable $M^{(i)}$. Indeed, we can write

$$P(M^{(1)}, \ldots, M^{(d)}) = \sum_{n = (n_1, \ldots, n_d)} P_n(M^{(1)}, \ldots, M^{(d)}),$$

where $P_n$ is homogeneous of degree $n_i$ in the matrix variable $M^{(i)}$. Since the space of homogeneous polynomials of multidegree $n$ is invariant under $GL(D)$, and spaces of different multidegree are linearly independent, each $P_n$ is $G$-invariant. Thus we may without loss of generality assume that $P = P_n$. Next, we reduce to multilinear invariants of some possibly larger number of matrices, as follows. Consider

$$P(M^{(1)}, \ldots, M^{(1), n_1}, \ldots, M^{(d), n_d}) = \sum_{h = (h_1, \ldots, h_d, n_d)} P_h(M^{(1), n_1}, \ldots, M^{(d), n_d}),$$

where $P_h$ is homogeneous of degree $h_1 \ldots h_d$ in each variable $M^{(i,j)}$. Now note that for all $t_1, 1, \ldots, t_d, n_d$

$$P \left( \sum_{i_1=1}^{n_1} t_{1,i_1} M^{(1,i_1)}, \ldots, \sum_{i_d=1}^{n_d} t_{d,i_d} M^{(d,i_d)} \right) = \sum_h t^h P_h(M^{(1), n_1}, \ldots, M^{(d), n_d}),$$

so if we take $M^{(i,j)} \equiv M^{(i)}$ for all $i \in [d]$ and $j \in [n_i]$ we have

$$P \left( \sum_{i_1=1}^{n_1} t_{1,i_1} M^{(1)}, \ldots, \sum_{i_d=1}^{n_d} t_{d,i_d} M^{(d)} \right) = \sum_h t^h P_h(M^{(1)}, \ldots, M^{(d)}).$$

On the other hand, by multihomogeneity,

$$P \left( \sum_{i_1=1}^{n_1} t_{1,i_1} M^{(1)}, \ldots, \sum_{i_d=1}^{n_d} t_{d,i_d} M^{(d)} \right) = \sum_h t^h P_h(M^{(1)}, \ldots, M^{(d)}).$$

Comparing coefficients and specializing to $h = (1, \ldots, 1)$, we find that

$$P(M^{(1)}, \ldots, M^{(d)}) = \frac{1}{n_1! \ldots n_d!} P_1(..., M^{(1)}, \ldots, M^{(1)}, \ldots, M^{(d)}, \ldots, M^{(d)}).$$

Note that $P_1,...,1$ is a multilinear polynomial in $\sum_{i=1}^d n_i$ matrix variables. Since the left-hand side of Eq. (IV.7) is $G$-invariant, we may also assume that $P_1,...,1$ is $G$-invariant. \square
We now return to our setting, where \( G = \text{GL}(D_1) \times \cdots \times \text{GL}(D_m), \) and use this lemma to prove.

**Proposition IV.13.** The ring \( \mathbb{C}[\text{Mat}_{d_1} \times \cdots \times \text{Mat}_{d_m}]^G \) of invariant polynomials is generated by functions \( P_{\pi,i} \) as in Eq. (IV.3) for \( n \leq \exp(c m D^2 \log(mD)) \) where \( D = \max(D_1, \ldots, D_m) \) and \( c > 0 \) is a universal constant.

**Proof.** Consider \( P = P(T^{(1)}, \ldots, T^{(d)}) \) as an element of \( \mathbb{C}[\text{Mat}_{d_1} \times \cdots \times \text{Mat}_{d_m}]^G. \) By Lemma IV.12 with \( D = D_1 \ldots D_m, \) we may reduce to the case where \( P = P_n \) for some \( n = (n_1, \ldots, n_d), \) and we can write

\[
P(T^{(1)}, \ldots, T^{(d)}) = \langle R, T^{(1)}, \ldots, T^{(1)} \rangle \otimes \cdots \otimes \langle R, T^{(d)}, \ldots, T^{(d)} \rangle,
\]

where \( \langle \cdot, \cdot \rangle \) is the trace inner product and where

\[
R \in (\text{End}((\mathbb{C}[D_1] \otimes \cdots \otimes \mathbb{C}[D_m])^G)^n).
\]

The total degree is given by \( n = \sum_{i=1}^{d} n_i. \) Now note that

\[
\left( \text{End}((\mathbb{C}[D_1] \otimes \cdots \otimes \mathbb{C}[D_m])^G)^n \right)^G 
\approx \text{End}((\mathbb{C}[D_1] \otimes \cdots \otimes \mathbb{C}[D_m])^G)^G
\approx \mathbb{C}[R_{\pi,i} : \pi_1 \in S_n] \otimes \cdots \otimes \mathbb{C}[R_{\pi,m} : \pi \in S_n]
\approx \mathbb{C}[R_{\pi,i} : \pi_1 \in S_n, \ldots, \pi_m \in S_n],
\]

where we denote by \( R_{\pi,i} \) the operator acting on \((\mathbb{C}[D_k])^n\) permuting the \( n \) copies of \( \mathbb{C}[D_k] \) according to \( \pi_k. \) Thus, \( R \) is a linear combination of elements of the form \( R_{\pi} = R_{\pi_1} \otimes \cdots \otimes R_{\pi_m}, \) for \( \pi = (\pi_1, \ldots, \pi_m). \) We conclude that the ring of invariant polynomials \( \mathbb{C}[\text{Mat}_{d_1} \times \cdots \times \text{Mat}_{d_m}]^G \) is generated as a vector space by the polynomial functions \( P_{\pi,i} \) as in Eq. (IV.3) for \( \pi \in S_n^m \) and \( n \in \mathbb{N}. \) In particular, the invariant polynomials of degree at most \( r \) spanned by the \( P_{\pi,i} \) for \( \pi \in S_n^m \) and \( i \in [d]^m \) for \( n \leq r. \)

We now use general results in invariant theory to bound the degree necessary to generate the invariant ring as an algebra. For convenience, we write \( V := \text{Mat}_{d_1} \times \cdots \times \text{Mat}_{d_m} \) so we are interested in degree bounds for the action of \( G = \text{GL}(D_1) \times \cdots \times \text{GL}(D_m) \) on \( V^d := \text{Mat}_{d_1} \times \cdots \times \text{Mat}_{d_m}. \) We first appeal to a classical theorem by Weyl [86, II.5 Thm. 2.5.A] which states that if \( d > \dim(V) \), a generating set of invariants for \( V^d \) can be obtained by acting with \( GL(D) \) on a generating set for \( \mathbb{C}[[V^d]] \rightarrow \mathbb{C}[[V^d]]^G \) (cf. [85, §7.1]). In particular, any degree bound for \( d = \dim(V) \) also applies to \( d > \dim(V) \). Accordingly, we may assume without loss of generality that \( d \leq \dim(V) \). Next, we observe that since we act by simultaneous conjugation, the invariants for the action of \( G \) are the same as for \( G' := \text{SL}(D_1) \times \cdots \times \text{SL}(D_m), \) so we can restrict to the latter. By results of Derksen [61] the ring of invariants is generated by invariant polynomials of degree at most

\[
r \leq \frac{3}{8} \dim(V^d)(H_{t}^{\dim(G')} A^{\dim(G')} )^2
\]

where \( t, H, A \) are integers computed as follows. We think of \( G' \) as being embedded in \( \bigoplus_{k=1}^{m} \text{Mat}_{D_k} \times D_k \cong \mathbb{C}^t, \) with \( t = \sum_{k=1}^{m} D_k^2. \) Then \( G' \) is defined as the common zero set of the polynomials \( \det(g_k) - 1 \) for \( k \in [m] \). The integer \( H \) is the maximal degree of these polynomials, i.e., \( H = \max_{k} D_k. \) If one fixes an arbitrary basis of \( V^d \), the matrix entries of the representation of \( G' \) are polynomial functions of the coordinates of \( G' \) (that is, the entries of the \( g_k \)). The integer \( A \) is the maximal degree of these polynomials. To compute it, note that \((g_1, \ldots, g_m) \in G' \) acts on a matrix tuple \( T = (T^{(i)})_{i=1}^{d} \in V^d \) by simultaneous conjugation by \( g_1 \otimes \cdots \otimes g_m. \) Thus, we left multiply each matrix \( T^{(i)} \) with \( g_1 \otimes \cdots \otimes g_m, \) the entries of which are polynomials of degree \( m \) in the entries of the \( g_k \), and we right multiply each \( T^{(i)} \) with

\[
g_1^{-1} \otimes \cdots \otimes g_m^{-1} = \text{adj}(g_1) \otimes \cdots \otimes \text{adj}(g_m),
\]

(IV.9)

where \( \text{adj}(g_k) \) is the adjugate matrix of \( g_k \) (here we used that \( g_k \in \text{SL}(D_k), \) so that we did not have to divide by the determinant when computing the inverse); since the entries of the adjugate matrix are given by cofactors of \( g_k \) and hence have degree \( D_k - 1 \), the entries of (IV.9) are polynomials of degree \( \sum_{k=1}^{m} (D_k - 1) = \sum_{k=1}^{m} D_k \).

Evaluating Eq. (IV.8) with \( \dim(V) = d \prod_{k=1}^{m} D_k^2, \) \( d \leq \dim(V), \) \( \dim(G') = \sum_{k=1}^{m} (D_k^2 - 1) \), \( H = \max_{k} D_k, \) \( t = \sum_{k=1}^{m} D_k^2 \) and \( A = \sum_{k=1}^{m} D_k \) shows that we can bound the required degree \( n \) by

\[
\frac{3}{8} \left( d \prod_{k=1}^{m} D_k^2 \right) \left( \max_{k} D_k \right)^m \left( \sum_{k=1}^{m} (D_k^2 - 1) \right)^2 \leq \exp(c m D^2 \log(mD))
\]

for some universal constant \( c \geq 0. \)

**Proof of Theorem IV.11.** It is clear that \( 1 \Rightarrow 2 \Rightarrow 3. \) The fact that \( 3 \Rightarrow 1 \) is a consequence of Proposition IV.13 and Theorem II.9.

**Corollary IV.14 (Lifting symmetries).** Suppose that \( S, T \in \text{Mat}_{D_1} \times \cdots \times \text{Mat}_{D_m} \) are in minimal canonical form and \( u \in \text{U}(d) \) is a unitary such that \( u_{\otimes m} | S_{\pi} \rangle = | T_{\pi} \rangle \) for all \( \pi \in S_n^m \) and \( n \in \mathbb{N}. \) Then there exist unitaries \( U_k \in \text{U}(D_k) \) such that \( (I \otimes u) | S \rangle = ((\bigotimes_{k=1}^{m} U_k \otimes \bar{U}_k) \otimes I) | T \rangle. \)

**Proof.** Let \( S' \in \text{Mat}_{D \times D} \) be the matrix tuple defined by

\[
| S' \rangle := (I \otimes u) | S \rangle.
\]

Then \( S' \) is also in minimal canonical form, since \( u \) is unitary and hence we have \( | g \cdot S' \rangle = | g \cdot S \rangle | S \rangle \) for all \( g \in G. \) Moreover, by construction it holds that

\[
| S'_{\pi} \rangle = u_{\otimes m} | S_{\pi} \rangle = | T_{\pi} \rangle
\]

for all \( \pi \in S_n^m \) and \( n \in \mathbb{N}. \) Thus Theorem IV.11 shows that \( S' \) and \( T \) are gauge equivalent, and it follows from Theorem IV.7 that there exist unitary gauge transformations \( U_k \in \text{U}(D_k) \) such that \( (I \otimes u) | S \rangle = ((\bigotimes_{k=1}^{m} U_k \otimes \bar{U}_k) \otimes I) | T \rangle. \)
The degree bounds in Proposition IV.13 are a direct consequence of deep and completely general results in invariant theory. These bounds are in general not necessarily sharp. As an example, the degree bounds obtained in this way for the MPS case are still exponential, while we know from Theorem III.13 that in this special case we have a degree bound of $D^2$. Moreover, we know from Remark III.15 that in this case invariants of degree $O(D)$ already suffice to determine whether two MPS tensors are gauge equivalent.

However, this is quite special for one spatial dimension. For PEPS with spatial dimension $m \geq 2$, we now show that one in general needs to consider invariants of degree exponential in the bond dimension in order to decide whether two PEPS tensors are gauge equivalent (even if one is the zero tensor). For convenience we take $m = 2$, $D_1 = D_2 = D$, and $d = 1$ (that is, the tensor networks defined by the PEPS tensors are scalars).

**Proposition IV.15 (Degree lower bound).** There exists a function $n_{\min}(D) = \exp(\Omega(D))$ and, for every $D$, a tensor $T \in \text{Mat}_{D^2 \times D^2}$ with the following properties:

1. For any invariant $P \in \mathbb{C}[\text{Mat}_{D^2 \times D^2}]^{GL(D) \times GL(D)}$ of degree less than $n_{\min}(D)$, we have $P(T) = P(0)$.
2. There exists an invariant polynomial of degree $n_{\min}(D)$ such that $P(T) \neq P(0)$. In particular, we have $0 \notin GL^{-1}T$, meaning that $T$ is not gauge equivalent to the zero tensor.

This means in particular that the ring of invariant polynomials $\mathbb{C}[\text{Mat}_{D^2 \times D^2}]^{GL(D) \times GL(D)}$ for any $d \geq 1$ is not generated by the polynomials of degree $n < n_{\min}(D)$.

**Proof.** The last statement of the proposition is an immediate consequence of the described properties of $T$. Indeed, if the ring of invariants were generated by invariant polynomials of degree smaller than $n_{\min}(D)$, then $P(T) = P(0)$ for all such polynomials $P$ would imply that $P(T) = P(0)$ for all invariant polynomials $P$ – but we know that $P(T) \neq P(0)$ for at least one invariant polynomial of degree $n_{\min}(D)$.

We will explicitly construct a tensor $T \in \text{Mat}_{D^2 \times D^2}$. For $d = 1$ and for $\pi \in S_n^m$ and $1 = (1, \ldots, 1)$ we abbreviate $P_{\pi, 1} = P_{\pi}$. Since the $P_{\pi}$ for $\pi \in S_n^2$ for $n < r$ are homogeneous and span the degree $r$ polynomials in $\mathbb{C}[\text{Mat}_{D^2 \times D^2}]^{GL(D) \times GL(D)}$ it suffices to show that $P_{\pi}(T) = 0$ for $\pi \in S_n^2$ for $n < n_{\min}$, while there exists some $\pi \in S_n^2$ for $n = n_{\min}$ such that $P_{\pi}(T) \neq 0$. We will take $n_{\min} = 2D^2 + D^2 - 2$.

To explain the construction and the argument we start with a construction where we allow the physical dimension $d$ to grow with $D$, and we construct a tensor $S \in \text{Mat}_{D^{2D-1}}$ with certain properties. Then, we will use a trick to reduce the physical dimension. Let $(|j\rangle |j\rangle)_{j=0}^{D-1}$ denote the standard basis of $\mathbb{C}^D$. We choose the tensor $S$ as follows:

$S^{(1)} = |0\rangle (|1\rangle \otimes |0\rangle) (|1\rangle$  

$S^{(2)} = |j\rangle (|0\rangle \otimes |j\rangle)$  

$S^{(2j+1)} = |0\rangle (|j+1\rangle \otimes |j\rangle$ $|j+1\rangle$  

for $j = 1, \ldots, D - 1$ and where the index $j$ should be read modulo $D$ (so $|D\rangle = |0\rangle$). We will now argue that one the one hand, for all $i = (i_1, \ldots, i_n) \in [2D - 1]^n$ and $n < 2D + 2^{D-1} - 2$ we have $P_{\pi, i}(S) = 0$ for all $\pi$, while on the other hand for $n = 2D + 2^{D-1} - 2$ there is some $\pi$ and $i = (i_1, \ldots, i_n)$ with $P_{\pi, i}(S) \neq 0$.

We start by showing that if $i = (i_1, \ldots, i_n)$ with $n < 2D + 2^{D-1} - 2$ then we have $P_{\pi, i}(S) = 0$. To conveniently reason about contractions in the tensor network picture we will name the four virtual legs of the tensors as follows:

[left] (right) \otimes (down) (up)

and call the two directions ‘horizontal’ and ‘vertical’. In the tensor network picture, we observe that for each even $i = 2j$ one can only contract the upper leg of $S^{(2j)}$ along the vertical direction with a copy of $S^{(2j+1)}$ in order for the result to be nonzero. That is, if we have $i_k = 1$, then $\pi_2$ must map $k$ to $l$ where $l = i + 1$. Similarly, for $i = 2j + 1 < 2D - 1$ odd we need to contract the right leg of $S^{(2j+1)}$ with the left leg of a copy of $S^{(2j+2)}$ in the horizontal direction and its upper leg with a copy of $S^{(2j+3)}$ in the vertical direction. Together these conditions imply that if $n_i$ denotes the number of copies of $S^{(i)}$ one requires in order for the contraction to be nonzero, we have $n_{i+2} \geq n_{i+1} + n_{i}$ for $i < 2D - 1$ odd and $n_{i+2} \geq n_{i}$ for $i \leq 2D$ even. By similar reasoning, for even $i = 2j$, the left leg of a copy of $S^{(2j)}$ needs to be contracted in the horizontal direction with a copy of $S^{(2j-1)}$ and, for odd $i = 2j + 1 > 1$, the down leg of a copy of $S^{(2j+1)}$ needs to be contracted in the vertical direction with a copy of $S^{(2j)}$ or $S^{(2j-1)}$. This implies that if $n_i \neq 0$ for $i \geq 2$ we also need either $n_{i-1}$ or $n_{i-2}$ to be nonzero and in particular $n_1 \geq 1$.

Solving the recursion with $n_1 \geq 1$ gives $n_{2i+1} \geq 2^i$ and $n_{2i} \geq 2^{i-1}$ for $i = 1, \ldots, D - 1$. We then have

$$n = \sum_{i=1}^{2D-1} n_i \geq 2D + 2^{D-1} - 2.$$  

On the other hand, it is easy to see that if we take $n$ copies of $S^{(i)}$ with $n_1 = 1$, $n_{2i+1} = 2^i$ and $n_{2i} = 2^{i-1}$ we can indeed contract to something nonzero.

Now, to prove the proposition, we adapt the previous construction to $d = 1$. We construct $T \in \text{Mat}_{D^2 \times D^2}$ as

$$T = T^{(1)} = \sum_{i=1}^{2D-1} S^{(i)}.$$  

Consider some arbitrary $\pi \in S_n^m$. We may expand $T = \sum_i S^{(i)}$ for each copy of $T$ to find

$$P_{\pi}(T) = \sum_{i \in [d]^n} P_{\pi, i}(S).$$  

By construction of $S$, each $P_{\pi, i}(S)$ is either zero or one, proving that $P_{\pi}(T) = 0$ if and only if there is some $i = (i_1, \ldots, i_n)$ such that $P_{\pi, i}(S) \neq 0$.

By our previous arguments for $S$ this implies that for all $n < 2D + 2^{D-1} - 2$ and $\pi \in S_n^m$ we have $P_{\pi}(T) = 0$, but
that for \( n = 2^D + 2^{D-1} - 2 \) we can find some \( \pi \in S_m \) such that \( P_\pi (T) \neq 0 \).

**Remark IV.16.** The argument of Proposition IV.15 can be extended to \( m > 2 \). We define a generalization of \( S \in \text{Mat}_{m(D-1)+1}^{m(D-1)+1} \) as follows: for \( i = 1, \ldots, D - 1 \) and \( j = 1, \ldots, m - 1 \) set

\[
S^{(1)} = (|0\rangle \langle 1|)^{\otimes m} \quad S^{(m(i-1)+j+1)} = (|0\rangle \langle 0|) \otimes |i\rangle \otimes (|0\rangle \langle i|)^{\otimes (m-j)},
\]

and

\[
S^{(mi+1)} = (|0\rangle \langle i+1|)^{\otimes (m-1)} \otimes |i\rangle \langle i+1|.
\]

Note that as before we interpret the basis states modulo \( D \), i.e., \( |D\rangle = |0\rangle \). Then again define \( T \in \text{Mat}_{mD^m}^{mD^m} \) by

\[
T = T^{(1)} = \sum_{i=1}^{m(D-1)+1} S^{(i)}.
\]

Essentially the same argument yields

\[
n_{\min} = 1 + \sum_{i=1}^{D-1} 2^{i(m-1)} \sum_{j=0}^{m-1} 2^j = \exp(\Omega(mD))
\]

so the degree lower bound also scales exponentially in \( m \).

We note here that proving degree lower bounds is not often an easy task, and in literature often has to employ rather involved and indirect techniques to get exponential lower bounds even in very familiar cases, see e.g., [87], [88]. The technique we use above is far more straightforward and explicit even though the setting we study here is somewhat similar to some of the cases handled in the aforementioned papers.

**D. Two-dimensional tensor networks, tilings and topology**

Consider the following question: given a PEPS tensor \( T \) in two spatial dimensions, determine whether there exist \( n_1, n_2 \) such that the associated state \( |T_{n_1,n_2}\rangle \) on a rectangular periodic lattice of size \( n_1 \times n_2 \) is nonzero. This problem is undecidable, see [28]. The proof of the undecidability given in [28] is by reducing to the problem of the existence of a periodic tiling given some set of tiles. Given a set of square tiles where each edge of the tile is associated to one of \( D \) boundary colors, the question is whether there exists a tiling (meaning that the boundary colors of adjacent tiles match) which is periodic. Equivalently, this gives a tiling of the two-dimensional torus. It is known that the existence of such tilings, given a set of tiles, is undecidable in general [89], and in [28] it was shown how to embed this problem into a PEPS tensor \( T \) of bond dimensions \( D_1 = D_2 = D \) such that the associated state \( |T_{n_1,n_2}\rangle \) on a \( n_1 \times n_2 \) periodic rectangular lattice is nonzero if and only if there exists a \( n_1 \times n_2 \) periodic tiling. The construction of such a tensor \( T \) is as follows. Let \( d \) be the number of tiles, label the tiles with an index \( i \in [d] \), and similarly label the colors with an index \( j \in [D] \). Then if the tile \( i \) has colors \( j_1, j_2, j_3, j_4 \) on respectively the left, right, upper and lower sides, define \( T^{(i)} := |j_1\rangle \langle j_2| \otimes |j_3\rangle \langle j_4| \). It is not very hard to see that under this construction the resulting PEPS state \( |T_{n_1,n_2}\rangle \) is nonzero if and only if there exists a \( n_1 \times n_2 \) periodic tiling. In fact, the argument in [28] is for PEPS tensors with boundary conditions, but the undecidability of the existence of periodic tilings [89] yields the same result for PEPS with periodic boundary conditions.

Interestingly, Proposition IV.13 shows that if one relaxes the problem to asking whether a PEPS tensor yields the zero state on any contraction graph, the problem is decidable, as we only have to check all graphs of size at most \( \exp(\Omega(D^2 \log D)) \). Alternatively, the PEPS tensor yields the zero state on any contraction graph if and only if its minimal canonical form is the zero tensor. In the language of invariant theory, the PEPS tensor yields the zero state on any contraction graph if and only if it is in the null cone.

**Example IV.17.** The following is the smallest set of tiles that only gives aperiodic tilings, meaning that if we take any rectangle with periodic boundary conditions, the associated PEPS equals zero [90].

In general, Proposition IV.13 together with the reduction in [28] shows that given a set of \( D \) colors, there exists a ‘generalized tiling’ (i.e. an arbitrary way to glue together the edges of the tiles) on some closed (possibly non-orientable) surface if and only if such a generalized tiling exists using at most \( \exp(\Omega(D^2 \log D)) \) tiles. The problem of deciding, given a set of \( D \) tiles, whether there exists some generalized tiling is thus a decidable problem. The construction in Proposition IV.15 in fact used a PEPS corresponding to a tiling problem, showing that there are indeed situations where the smallest possible generalized tilings are of size at least \( \exp(\Omega(D)) \).

As argued in [28] their undecidability result excludes the possibility of a computable canonical form for two-dimensional PEPS which is such that two tensors \( T, S \) yield the same state on all periodic lattices (so \( |T_{n_1,n_2}\rangle = |S_{n_1,n_2}\rangle \) for all \( n_1, n_2 \)) if and only if they have the same canonical form. On the other hand, we saw in Corollary IV.9 that any two normal tensors which yield the same state on a periodic lattice are related by a local gauge transformation. However, even if generic tensors are normal, in two spatial dimensions many interesting...
tensors describing physical systems are not normal, in particular those associated to topological order, either conventional or symmetry-protected [14]. One way to interpret our Fundamental Theorem (Theorem IV.11) is that for some tensors it does not suffice to place them on periodic lattices and that the state they describe has a type of topological order which is only revealed by placing the states on a (possibly non-orientable) two-dimensional manifold other than a torus. This is an idea which is worth exploring in the future, and it is reminiscent of the well-known fact that different topological sectors can be detected by imposing different boundary conditions [14].

E. When does one need the orbit closure?

In general, finding the minimal canonical form requires one to go to the closure of the orbit of the action by the gauge group. In other words, if $T \in \text{Mat}_{D_1 \times \ldots \times D_n}^d$ is a PEPS tensor in $m$ spatial dimensions, then there may not exist a minimal canonical form $T_{\text{min}}$ of the form $(g_1, \ldots, g_m) \cdot T$, but only one that can be written as a limit of such tensors: $T_{\text{min}} = \lim_{m \to \infty} (g_1, \ldots, g_m) \cdot T$. When is this really necessary? In this section we will discuss conditions under which one does not need to go to the closure and give an example where it is required. We consider PEPS tensors in $m$ spatial dimensions, and fix bond dimensions $D_1, \ldots, D_m$ and physical dimension $d$. We denote by $G = \text{GL}(D_1) \times \cdots \times \text{GL}(D_m)$.

We will now argue that given $S \in \text{Mat}_{D_1 \times \ldots \times D_n}^d$ in minimal canonical form, if there exists a $T$ which has $S$ as a canonical form and which requires taking an orbit closure, then the tensor $S$ must have a continuous symmetry. We formalize the notion of a continuous symmetry by a multiplicative one-parameter subgroup of $G$, which is a homomorphism of Lie groups $\phi : \mathbb{C}^* \to G$. Given such a homomorphism we will write $g(z)$ for $\phi(z)$ and we will say that $g(z)$ is nontrivial if $g(z)$ is not proportional to the identity for all $z \in \mathbb{C}^*$.

The result we are aiming for is a consequence of the Hilbert-Mumford criterion in geometric invariant theory. If $T \in \text{Mat}_{D_1 \times \ldots \times D_n}^d$ is any tensor, and $T_{\text{min}}$ is an associated minimal canonical form, then $G \cdot T_{\text{min}}$ is a closed orbit (by the Kempf–Ness Theorem, see Theorem II.5). The Hilbert-Mumford criterion (see for instance Theorem 3.24 in [40]) then implies that there exists a one-parameter subgroup $g(z) \in G$ such that

$$\lim_{z \to 0} g(z) \cdot T = S$$

where $S \in G \cdot T_{\text{min}}$.

**Proposition IV.18** (Non-closed implies symmetry). Suppose $S \in \text{Mat}_{D_1 \times \ldots \times D_n}^d$ is such that $G \cdot S$ is closed (in particular this is valid if $S$ is in minimal canonical form). Suppose that there exists $T$ such that $S \in G \cdot T$ but $S \notin G \cdot T$, then there exists a nontrivial one-parameter subgroup $g(z) \in G$, $z \in \mathbb{C}^*$ such that $g(z) \cdot S = S$ for all $z \in \mathbb{C}^*$.

**Proof.** By the Hilbert-Mumford criterion there exists $g \in G$ and a one-parameter subgroup $h(z) \in G$ such that

$$\lim_{z \to 0} h(z) \cdot T = g \cdot S.$$ 

This one-parameter subgroup must be nontrivial since $S \notin G \cdot T$. Let $g(z) = g^{-1} h(z) g$. Then

$$g(z) \cdot S = g^{-1} h(z) g \cdot S = \lim_{w \to 0} g^{-1} h(z) h(w) \cdot T = \lim_{w \to 0} g^{-1} h(z w) \cdot T = g^{-1} \cdot (g \cdot S) = S$$

confirming that $g(z)$ is a symmetry for $S$.

**Example IV.19.** Returning to the GHZ state in Example III.4, we note that it indeed has a one-parameter subgroup symmetry, for instance for

$$g(z) = \begin{pmatrix} 1 & 0 \\ 0 & z \end{pmatrix}$$

it holds that $g(z) \cdot M = M$.

An important class of examples of PEPS tensors which lead to closed orbits are injective and normal tensors, already defined in Section IV-B. For those tensors (in particular for normal MPS) one does not need to take closures to construct the minimal canonical form. In fact we show that if there is any normal tensor in $G \cdot T$, then $G \cdot T$ is closed (and in particular contains a minimal canonical form for $T$). A similar result has been shown for the case of MPS in [85] and has applications in the classification of two-dimensional SPT phases. This is a nice example where the geometric invariant theory framework allows for a particularly simple and conceptually elegant proof.

**Proposition IV.20** (Canonical form normal PEPS). Suppose $T \in \text{Mat}_{D_1 \times \ldots \times D_n}^d$ is such that its orbit closure $G \cdot T$ contains a normal tensor. Then $G \cdot T = G \cdot T$.

**Proof.** By Proposition IV.18 it suffices to show that if $T$ is normal, then $G \cdot T$ is closed and there is no nontrivial one-parameter subgroup $g(z)$ such that $g(z) \cdot T = T$ for all $z \in \mathbb{C}^*$.

Let $T$ be the $n = n_1 \times \cdots \times n_m$ blocking of $T$ such that $T$ is injective. So, if we let $D_i = D_i^{n_1 \times \cdots \times n_{i-1} \times 1 \times n_{i+1} \times \cdots \times n_m}$ and $d = d^0$,

$$T \in \text{Mat}_{D_1 \times \cdots \times D_n}^d.$$

Let $S$ be any tensor in $G \cdot T$ and let $S$ be the $n_1 \times \cdots \times n_m$ blocking of $S$. Since $S \in G \cdot T$ there must be a sequence $g^{(j)} = (g^{(j)}_1, \ldots, g^{(j)}_m) \in G$ for $j \in \mathbb{N}$ such that

$$\lim_{j \to \infty} g^{(j)} \cdot T = S.$$

Since $g \cdot T$ is invariant under rescaling the $g_k$ by a constant, we may assume that $\|g^{(j)}_k\| = 1$ for all $k$ and $j$. If we let $g^{(j)}_k = (g^{(j)}_k)^{n_1 \times \cdots \times n_{i-1} \times 1 \times n_{i+1} \times \cdots \times n_m}$ and $g^{(j)} = (g^{(j)}_1, \ldots, g^{(j)}_m)$ then

$$\lim_{j \to \infty} g^{(j)} \cdot T = S.$$

Now, interpret $T$ as an element of $(\mathbb{C}^D \otimes \mathbb{C}^D)^{d^0}$ where $D = D_1 \cdots D_m$, so

$$T = (T^{(i)})^{d^0}_{i=1}, \quad T^{(i)} \in \mathbb{C}^{D_i} \otimes \mathbb{C}^{D_i}.$$
Then the fact that $\tilde{T}$ is injective implies that there exists a tensor $\hat{M} \in (\mathbb{C}^{D} \otimes \mathbb{C}^{D})^{d}$ which is an inverse to $\tilde{T}$ in the sense that

$$
\sum_{i=1}^{d} \tilde{T}^{(i)}(\hat{M}^{(i)})^{\dagger} = I_{D^{d}}
$$

is the identity map. Let $\tilde{N}^{(i)}$ be the contraction of $\tilde{g}^{(j)} \cdot \tilde{T}$ with $\hat{M}$:

$$
\tilde{N}^{(j)} = \sum_{i=1}^{d} \left( \tilde{g}^{(j)} \otimes (\tilde{g}^{(j)})^{-T} \tilde{T}^{(i)} \right) (\hat{M}^{(i)})^{\dagger}
$$

(writing $\tilde{g}^{(j)} = g_{1}^{(j)} \otimes \ldots \otimes g_{m}^{(j)}$ in a slight abuse of notation). Then, $\tilde{N}^{(j)}$ must be a converging sequence (since $\tilde{g}^{(j)} \cdot \tilde{T}$ is so). On the other hand, since $\hat{M}$ is the inverse to $\tilde{T}$,

$$
\tilde{N}^{(j)} = \tilde{g}^{(j)} (\tilde{g}^{(j)})^{-T}.
$$

The fact that this sequence converges implies that the norm $\| (\tilde{g}^{(j)})^{-T} \|_{\infty} = \| (\tilde{g}^{(j)})^{-1} \|_{\infty}$ is bounded and hence there is some constant $C$ such that for all $k \in [m]$ and $j \in \mathbb{N}$ we may bound $\| (g_{k}^{(j)})^{-1} \|_{\infty} \leq C$. However, this implies that $g^{(j)}$ is contained in a compact subset of $G$ and therefore has a converging subsequence, which in turn implies that

$$
S = \lim_{j \to \infty} g^{(j)} \cdot T \in G \cdot T.
$$

So, we conclude that $G : T$ is closed. Secondly, suppose that there exists a nontrivial one-parameter subgroup $g(z)$ such that $g(z) \cdot T = T$ for all $z \in \mathbb{C}^{*}$. Using the same notation as before, this implies that there exists a one-parameter subgroup $\tilde{g}(z)$ such that $\tilde{g}(z) \cdot \tilde{T} = \tilde{T}$. However, applying the inverse $\hat{M}$, this implies

$$
\tilde{g}(z) \cdot \tilde{g}(z)^{-T} = I
$$

which implies that $g(z)$ must be proportional to the identity for all $z \in \mathbb{C}^{*}$.

Beyond normal PEPS states there are also other states of interest where Proposition IV.18 implies that one never needs to go to the closure to obtain the minimal canonical form.

**Example IV.21.** In two spatial dimensions an important example of a PEPS state which is not normal is the toric code. This is a state usually defined on a qubit lattice. To write it as a PEPS state one may group together four physical sites into a single site of four qubits. The toric code PEPS tensor is then given, as a map from the bond legs to the physical legs, by $T = \frac{1}{2} I_{Z^{4}} + \frac{1}{2} Z^{4}$. Alternatively, for $i, j, k, l \in \{0, 1\}$

$$
T^{(i,j,k,l)} = \begin{cases} 
| i \rangle \langle j | \otimes | k \rangle \langle l | & \text{if } i + j + k + l \text{ is even}, \\
0 & \text{if } i + j + k + l \text{ is odd}.
\end{cases}
$$

This tensor is in minimal canonical form, since all virtual marginals are maximally mixed. We will now verify that this tensor has a finite symmetry group, and hence (as opposed to the GHZ state) there are no tensors for which $T$ is in their orbit closure while not in the orbit itself. Suppose that $g \cdot T = T$ for $g = (g_{1}, g_{2})$ with $g_{k} \in \text{GL}(2)$ for $k = 1, 2$. This is equivalent to

$$
g_{1} \otimes g_{1}^{-T} \otimes g_{2} \otimes g_{2}^{-T} | i \rangle \langle j | \langle k \rangle \langle l | = | i \rangle \langle j | \langle k \rangle \langle l | \cdot
$$

for all $i + j + k + l = 0 \mod 2$. We can choose $i$ and $j$ arbitrary, so $g_{1}$ must be diagonal. By the same reasoning, $g_{2}$ must be diagonal as well. If we let

$$
g_{i} = \begin{pmatrix} g_{i,0} & 0 \\ 0 & g_{i,1} \end{pmatrix}
$$

then we find $g_{i} g_{j} = g_{i,j} g_{j,i}$ for all $i + j + k + l = 0 \mod 2$. By choosing $i \neq j$ and $k \neq l$ it is easy to see that this implies that after scaling by a global constant (which is irrelevant) $g_{i,j} \in \pm 1$ so we cannot have a nontrivial one-parameter subgroup symmetry.

**Example IV.22.** The previous example can be generalized to arbitrary quantum double models for abelian groups $G$. For an arbitrary finite group $G$ we may construct a PEPS tensor (also known as a $G$-isometric PEPS tensor) as follows. The Hilbert space along each of the bond legs consists of the group algebra $\mathbb{C}[G]$ with basis $| g \rangle$, so the bond dimension is $D = |G|$. The group $G$ acts by the regular representation on $\mathbb{C}[G]$ as $g | h \rangle = | gh \rangle$. The physical Hilbert space is given by $\mathbb{C}[G]^{4}$. Then the PEPS tensor is given, as a map from the bond Hilbert spaces to the physical Hilbert space as

$$
T = \frac{1}{|G|} \sum_{g \in G} g \otimes \bar{g} \otimes g \otimes \bar{g}
$$

The toric code tensor is a special case of this construction for $G = \mathbb{Z}_{2}$. Essentially the same argument as for the toric code shows that (up to a global constant) the symmetries of this tensor form a discrete set if the group $G$ is abelian and hence $\mathbb{C}[G]$ decomposes into one-dimensional irreducible representations. Therefore, $\text{GL}(D) \times \text{GL}(D) \cdot T = \text{GL}(D) \times \text{GL}(D) \cdot T$.

**Example IV.23.** To give a nontrivial example where we do have a continuous symmetry, and we have non-closed orbits, we use a construction inspired by [91], which investigates PEPS with continuous virtual symmetries. Consider a 2-dimensional PEPS tensor $T$ with physical and bond dimensions all equal to two, given by

$$
T^{(0)} = \sum_{i,j \in \{0,1\}} | i \rangle \langle j | \otimes | i \rangle \langle j |,
$$

$$
T^{(1)} = \sum_{i,j \in \{0,1\}} | i \rangle \langle j | \otimes X | i \rangle \langle j | X.
$$

In the standard basis we may write this out as

$$
T^{(0)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad T^{(1)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.
$$

See [91] for a graphical notation, expressing contractions as loop diagrams. All the virtual marginals of $T$ are maximally mixed, so $T$ is in minimal canonical form. It is now easy
to see that $g(z) = (h(z), h(z))$ is a one-parameter subgroup symmetry for

$$h(z) = \begin{pmatrix} 1 & 0 \\ 0 & z \end{pmatrix}.$$ 

Indeed, since

$$h(z) |i⟩⟨j| h(z)^{-1} = z^{i-j} |i⟩⟨j|,$$

we find

$$(h(z) \otimes h(z)) T(0) (h(z)^{-1} \otimes h(z)^{-1}) = \sum_{i,j \in \{0,1\}} z^{i-j} |i⟩⟨j| \otimes z^{j-i} |j⟩⟨i| = T(0)$$

and

$$(h(z) \otimes h(z)) T(1) (h(z)^{-1} \otimes h(z)^{-1}) = \sum_{i,j \in \{0,1\}} z^{i-j} |i⟩⟨j| \otimes z^{j-i} X |i⟩⟨j| X = T(1).$$

Let us construct an explicit example where we need the closure to reach the minimal canonical form. Let $N = |1⟩⟨0| \otimes |1⟩⟨0|$ and let

$$S(0) = T(0) + N \quad \text{and} \quad S(1) = T(1) + N.$$ 

In the standard basis

$$S(0) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad S(1) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}.$$

Now, since $h(z) |1⟩⟨0| h(z)^{-1} = z |1⟩⟨0|$ and $T$ is invariant under $g(z)$,

$$(h(z) \otimes h(z)) S(i) (h(z)^{-1} \otimes h(z)^{-1}) = T(i) + z^2 N$$

so

$$\lim_{z \to 0} g(z) \cdot S = T.$$

On the other hand, since $1 = \text{rank}(T(1)) \neq \text{rank}(S(1)) = 2$ we see that $S$ is not in the orbit of $T$.

V. ALGORITHMS FOR COMPUTING MINIMAL CANONICAL FORMS

In this section we address the question of how to compute minimal canonical forms algorithmically. We will discuss two algorithms (and sketch potential applications in Section VI). The first one is eminently practical and stated explicitly in Algorithm 1. The second one has a better runtime dependence in theory, but is less practical. Both algorithms have their origin in a series of recent works on norm minimization and scaling problems, in increasing generality, including matrix, operator and tensor scaling (see [51], [52], [54], [55], [57], [62], [63] and references therein). We follow and apply the general framework of [52] but give some tighter bounds in our setting.

Before discussing our results and presenting our algorithm in more detail, we discuss what it means to compute a minimal canonical form. In general, minimal canonical forms cannot be represented exactly in finite precision, so one is naturally led to look for approximations. Then there are at least three natural choices of what it might mean to approximately compute a minimal canonical form of a given PEPS tensor $T$:

- **ℓ2-error in the space of tensors**: Given $δ > 0$, find a tensor $S \in G \cdot T$ that is $δ$-close in ℓ2-norm to a minimal canonical form $T_{\text{min}}$ of $T$. It is natural consider relative error (but see Remark V.17):

$$\|S - T_{\text{min}}\|_2 \leq δ.$$  \hfill (V.1)

- **ℓ2-error in the first-order characterization**: Given $ε > 0$, find a tensor $S \in G \cdot T$ such that

$$\frac{1}{\text{tr} \, σ} \sum_{k=1}^m \|σ_k,1 - σ_T^{k,2}\|_2 \leq ε \quad \text{where} \quad σ = |S⟩⟨S|.$$  \hfill (V.2)

- **error in the norm of the tensor**: Given $ζ > 0$, find a tensor $S \in G \cdot T$ whose norm is almost minimal:

$$\frac{\|T_{\text{min}}\|_2}{\|S\|_2} \geq 1 - ζ.$$  \hfill (V.3)

We already know that Eq. (V.1) holds with $δ = 0$ if and only if Eq. (V.2) holds with $ε = 0$ and if only if Eq. (V.3) holds with $ζ = 0$ (by Theorem IV.8 and the definition of the minimal canonical form). In Section V-B we will show that the three error measures can be related in a precise way. Accordingly, we may target either, and we will see that Eqs. (V.2) and (V.3) arise naturally when designing approximation algorithms.

A. First-order algorithm

We start by motivating our first algorithm, which we present explicitly in Algorithm 1. Suppose we are given a tensor $T \neq T = (T(i)_{i=1}^d) \in \text{Mat}_{D_1 \ldots D_m} \times \ldots \times \text{Mat}_{D_1 \ldots D_m}$ and we would like to approximately compute a minimal canonical form $T_{\text{min}}$. Since the latter is defined as a minimum norm tensor in the orbit closure, a natural way to address this is by minimizing or “infimizing” the norm or, equivalently, one half the norm square

$$\frac{1}{2} \|g \cdot T\|_2^2$$

over $g \in G = \text{GL}(D_1) \times \ldots \times \text{GL}(D_m)$. Because the norm is invariant under the action of $K = U(D_1) \times \ldots \times U(D_m)$, the objective function

$$f_T(g) := \frac{1}{2} \|g \cdot T\|_2^2$$

only depends on the tuple $p = (g_1^1, g_1^2, \ldots, g_m^1, g_m^2)$ of positive definite matrices in $P = \text{PD}(D_1) \times \ldots \times \text{PD}(D_m)$. However, $P$ is not a convex subset of $H := \text{Herm}(D_1) \oplus \ldots \oplus \text{Herm}(D_m)$ and accordingly $\inf_{p \in P} f_T(p)$ is not a convex optimization problem that can be addressed by standard methods (e.g., by semidefinite programming)!

Instead, we proceed differently. Since $f_T(g) = f_T(ρg)$ for all $k \in K$ and $g \in G$, the objective function $f_T$ can be defined on the space $K \setminus G := \{ Kg : g \in G \}$ of
right $K$-cosets in the gauge group $G$. This space may be endowed with a natural Riemannian metric, yielding a simply-connected complete Riemannian manifold with non-positive curvature [92], [93]. In particular, between any two points there exist unique geodesics (here: shortest paths). Explicitly, the geodesics through $g = (g_1, \ldots, g_m) \in G$ take the form $K(e^{X_1}g_1, \ldots, e^{X_m}g_m)$ for $X = (X_1, \ldots, X_m) \in H$.

The point then is the following: While not convex in the ordinary sense, the function $f_T(p)$ is geodesically convex, that is, convex along these geodesics. This means for any $(g_1, \ldots, g_m) \in G$ and $(X_1, \ldots, X_m) \in H$,

$$\partial_2^{t=0} f_T(e^{X_1}g_1, \ldots, e^{X_m}g_m) \geq 0.$$

Therefore, a reasonable approach to minimizing $f_T$ is to use a gradient descent. What is the gradient in this setting at, say, $g = I = (I_{D_1}, \ldots, I_{D_m})$? The computation done in Eq. (IV.4)

shows that

$$\partial_2 f_T(e^{X_1}, \ldots, e^{X_m}) = \frac{1}{t} \partial_{t=0} \| (e^{X_1}, \ldots, e^{X_m}) \cdot T \|^2_2 = \sum_{k=1}^m \text{tr} [X_k (\rho_{k,1} - T_{k,2})].$$

where $\rho = [T] (T)$, and hence we should think of

$$\nabla f_T(I) = (\rho_{k,1} - T_{k,2})_{k=1}^m,$$

which is an element of $H = \text{Herm}(D_1) \oplus \cdots \oplus \text{Herm}(D_m)$, as the gradient at $g = I$! Accordingly, starting at $g = I$ and moving along the geodesic with this direction, we should take a gradient step of the form

$$T \mapsto g \cdot T$$

where

$$g := \left(e^{-\eta (\rho_{1,1} - T_{1,2})}, \ldots, e^{-\eta (\rho_{m,1} - T_{m,2})}\right).$$

for some suitable step size $\eta > 0$. Note that, crucially, this amounts to acting by the gauge group, i.e., will automatically remain in the $G$-orbit!

Now we have almost derived Algorithm 1, except for one observation: The function $f_T$ is not only convex along geodesics, but even log-convex! This gives stronger guarantees, so we consider

$$F_T(g) = \frac{1}{2} \log(2 f_T(g)) = \log \| g \cdot T \|_2,$$

with gradient

$$\nabla F_T(I) = \frac{1}{2 f_T(I)} (\rho_{k,1} - T_{k,2})_{k=1}^m = \frac{1}{\text{tr} \rho} (\rho_{k,1} - T_{k,2})_{k=1}^m.$$

Similar to the ordinary gradient descent in Euclidean space, under suitable hypotheses on a geodesically convex objective one can provide a “safe” choice for the step size $\eta$. In the present case, the objective $F_T$ is $4m$-smooth along geodesics: for every $g = (g_1, \ldots, g_m) \in G$ and $X = (X_1, \ldots, X_m) \in H$, one has

$$\partial_2^{t=0} f_T(e^{X_1}g_1, \ldots, e^{X_m}g_m) \leq 4m \| X \|_2,$$

where $\| X \|_2 = \sum_{k=1}^m \| X_k \|_2$. For such functions, $\eta = \frac{1}{4m}$ is a suitable step size and this is what we use in Algorithm 1. Below, we give formal guarantees for the performance of the algorithm. We remark that Theorem V.1 is a special case of [52, Thm. 4.2].

**Theorem V.1.** Let $T \in \text{Mat}_{D_1 \times \cdots \times D_m}$ be such that $T_{\text{min}} \neq 0$ (for some and hence for any minimal canonical form), and let $\varepsilon > 0$. Then Algorithm 1 outputs a group element $g \in \text{GL}(D_1) \times \cdots \times \text{GL}(D_m)$ such that the tensor $S := g \cdot T$ satisfies

$$\frac{1}{\text{tr} \sigma} \sum_{k=1}^m \| \sigma_{k,1} - T_{k,2} \|_2^2 \leq \varepsilon,$$

where $\sigma = |S \langle S|$, within $O(\frac{m}{\varepsilon \log \| T \|_2 / T_{\text{min}}})$ iterations.

**Proof.** We analyze Algorithm 1. For $t = 0, 1, 2, \ldots$ and $g^{(t)}$ the group elements produced by the algorithm. If the algorithm

---

**Algorithm 1:** Computing PEPS normal forms

**Input:** A uniform PEPS tensor $T \in \text{Mat}_{D_1 \times \cdots \times D_m}$ and $\varepsilon > 0$.

**Output:** A gauge transformation $g \in \text{GL}(D_1) \times \cdots \times \text{GL}(D_m)$.

1. $g^{(0)} \leftarrow (I_{D_1}, \ldots, I_{D_m})$;
2. for $t = 0, 1, \ldots$ do
3. $T^{(t)} \leftarrow g^{(t)} \cdot T$;
4. $\rho^{(t)} \leftarrow |T^{(t)} \langle T^{(t)}|$
5. if $\sum_{k=1}^m \| \rho^{(t)}_{k,1} - \rho^{(t)}_{k,2} \|_2^2 \leq \varepsilon^2$ then
6. return $g^{(t)}$;
7. end if
8. for $k = 1, \ldots, m$ do
9. $g^{(t+1)}_{k} \leftarrow e^{-\frac{1}{4m} \text{tr} \rho^{(t)}_{k,2}} (\rho^{(t)}_{k,1} - \rho^{(t)}_{k,2}) g^{(t)}_{k}$;
10. end for
11. end for

and updates

$$T \mapsto g \cdot T$$

where

$$g := \left(e^{-\eta (\rho_{1,1} - T_{1,2})}, \ldots, e^{-\eta (\rho_{m,1} - T_{m,2})}\right).$$


does not terminate in the $t$-th iteration, then we may estimate the difference $F_T(g^{(t+1)}) - F_T(g^{(t)})$, using Eq. (V.6) by

$$F_T(g^{(t+1)}) - F_T(g^{(t)}) = F_{T(I)}(e^{-\frac{1}{m}} \nabla F_{T(I)}(I)) - F_{T(I)}(I)$$

$$\leq tr \left[ \nabla F_{T(I)}(I) \cdot \left( -\frac{1}{4m} \nabla F_{T(I)}(I) \right) \right]$$

$$+ \frac{m}{8} - \frac{1}{m} \nabla F_{T(I)}(I) \right) ^2$$

$$= - \frac{1}{8m} \nabla F_{T(I)}(I) ^2 - \frac{\varepsilon^2}{8m},$$

where the first inequality follows since $F_T$ is a convex and $4m$-smooth function [52, Lemma 3.8]. Accordingly, if the algorithm has not terminated up to and including the $t$-th iteration, then

$$\log \left\| T_{\text{min}} \right\|_2 ^2 \leq \log \left\| g^{(t)} \cdot T \right\|_2 - \log \left\| T \right\|_2$$

$$= F_T(g^{(t)}) - F_T(g^{(0)}) < -t \frac{\varepsilon^2}{8m},$$

or

$$t < \frac{8m}{\varepsilon^2} \log \left\| T_{\text{min}} \right\|_2.$$

The iteration bound of Theorem V.1 involves $\left\| T_{\text{min}} \right\|_2$. If the entries of $T$ are given by some finite number of bits then this quantity can be estimated in an $a$ priori fashion, by first rescaling $T$ such that its entries are given by Gaussian integers, i.e., are in $\mathbb{Z}[i]$, and then using the following result.

**Proposition V.2.** Let $T \in \text{Mat}^{d} _{D_1 \cdots D_m \times D_1 \cdots D_m}$ with $T_{\text{min}} \neq 0$, and assume that all entries of $T$ are in $\mathbb{Z}[i]$. Then,

$$\left\| T_{\text{min}} \right\|_2 \geq \frac{1}{\prod_{j=1}^{m} D_j}.$$

**Proof.** We use the fact that the invariant ring is generated by the functions $P_{\pi,i}$ defined in Eq. (IV.3). Since $T_{\text{min}} \neq 0$, there exist $n \geq 1$, $\pi \in \mathbb{S}_n$ and $i \in [d]^n$ such that $P_{\pi,i}(T) \neq 0$. But $P_{\sigma,i}$ is a polynomial with integer coefficients in the entries of $T$; therefore, evaluating it on $T$ with entries in $\mathbb{Z}[i]$ must yield $|P_{\pi,i}(T)| \geq 1$. Furthermore, it is an invariant under the PEPS action, so we deduce for any $g \in G$:

$$1 \leq |P_{\pi,i}(T)| = |P_{\pi,i}(g \cdot T)|$$

$$= \left| \text{tr} \left[ (R_{\pi_1} \otimes \cdots \otimes R_{\pi_m})(g \cdot T^{(i_1)} \otimes \cdots \otimes (g \cdot T^{(i_m)}) ) \right] \right|$$

$$\leq \left\| R_{\pi_1} \otimes \cdots \otimes R_{\pi_m} \right\|_2 \cdot \left\| (g \cdot T^{(i_1)} \otimes \cdots \otimes (g \cdot T^{(i_m)}) \right\|_2.$$

Since each $R_{\pi_j}$ is unitary, the same is true of their tensor product. As it acts on a space of dimension $(\prod_{j=1}^{m} D_j)^n$, one obtains

$$\left\| R_{\pi_1} \otimes \cdots \otimes R_{\pi_m} \right\|_2 = \left( \prod_{j=1}^{m} D_j \right)^n.$$

Furthermore,

$$\left\| (g \cdot T^{(i_1)} \otimes \cdots \otimes (g \cdot T^{(i_m)}) \right\|_2 \leq \left( \max_i \left\| g \cdot T^{(i)} \right\|_2 \right)^n \leq \left\| g \cdot T \right\|_2 ^m.$$ Combining the two estimates, taking $n$-th roots and the infimum over $g \in G$ yields the desired estimate. $\square$

The above approach of evaluating an invariant to prove norm lower bounds is used in other settings as well, e.g., for tensor scaling in [63, Thm. 7.12], and for much more general actions in [52, Cor. 7.19]; but appealing to the latter result would result in a worse bound.

We obtain the following corollary, which implies an $\text{poly}(\frac{1}{\varepsilon}, \text{input size})$-algorithm, cf. [52, Rem. 8.1]:

**Corollary V.3.** Let $T \in \text{Mat}^{d} _{D_1 \cdots D_m \times D_1 \cdots D_m}$ be a tensor such that $T_{\text{min}} \neq 0$ (for some and hence for any minimal canonical form). Assume that the entries of $T$ are in $\mathbb{Q}[i]$ and given by storing the numerators and denominators in binary. Let $\varepsilon > 0$. Then Algorithm 1 outputs a group element $g \in \text{GL}(D_1) \times \cdots \times \text{GL}(D_m)$ such that the tensor $S := g \cdot T$ satisfies

$$\frac{1}{\text{tr} \sigma} \left\| \sum_{k=1}^{m} \left| \sigma_{k,1} - \sigma_{k,2} \right| \right\|_2 \leq \varepsilon,$$ where $\sigma = |S \rangle < S \rangle$.

within $O\left( \frac{1}{\varepsilon} \cdot \text{poly}(|\langle \rangle T \rangle) \right)$ iterations, where $\langle \rangle$ denotes the total number of bits used to represent $T$.

**B. Relation between approximation errors**

In Section V-A, we discussed three natural notions of approximation error in Eqs. (V.1) to (V.3), and we gave an algorithm targeting Eq. (V.2), i.e., given a tensor $T$ and $\varepsilon > 0$, we discussed how to obtain a tensor $S \in G \cdot T$ such that

$$\frac{1}{\text{tr} \sigma} \left\| \sum_{k=1}^{m} \left| \sigma_{k,1} - \sigma_{k,2} \right| \right\|_2 \leq \varepsilon,$$ where $\sigma = |S \rangle < S \rangle$.

We will now see that there is a precise quantitative relationship between these notions. As we will see, the following quantity will play a crucial role.

**Definition V.4.** Given bond dimensions $D_1, \ldots, D_m$, define $\gamma(D_1, \ldots, D_m) := \gamma$ by

$$\gamma := \begin{cases} \frac{1}{D_1^{1/2}}, & \text{if } m = 1, \\ \frac{1}{(2m+1)^{1/2}} \left( \sum_{i=1}^{m} D_i \right)^{-1/2}, & \text{if } m \geq 2. \end{cases}$$

Note that $\gamma$ is only inverse polynomially small in the bond dimension for $m = 1$, while it is exponentially small for $m \geq 2$. Then we have the following relation between Eqs. (V.2) and (V.3).

**Theorem V.5.** Let $0 \neq T \in \text{Mat}^{d} _{D_1 \cdots D_m \times D_1 \cdots D_m}$ and $S \in G \cdot T$. Then:

$$1 - \frac{\varepsilon}{\gamma} \leq \frac{\left\| T_{\text{min}} \right\|_2}{\left\| S \right\|_2} \leq 1 - \frac{\varepsilon^2}{8m},$$

for

$$\varepsilon := \frac{1}{\text{tr} \sigma} \left\| \sum_{k=1}^{m} \left| \sigma_{k,1} - \sigma_{k,2} \right| \right\|_2.$$

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where \( \sigma = |S]\langle S \rangle \) and \( \gamma \) is the constant defined in Definition V.4. In particular, if \( \varepsilon < \gamma \), then \( T_{\min} \neq 0 \).

We will prove Theorem V.5 by appealing to a non-commutative duality theorem given in [52, Thm. 1.17]. To explain how this theorem applies in our setting, we must define a complexity measure defined by combinatorial data associated with representations known as the weight margin. The parameter \( \gamma \) which appears in Definition V.4 is a lower bound on this weight margin. We shall do this using the language from Section II to make it easier to bridge the gap, and show how the definitions specialize for our representation.

Let \( \pi: G \to GL(V) \) be a representation of a group \( G \subseteq GL(n) \), where we make the same assumptions as in Section II. It is known that such \( G \) contains a maximal algebraic torus, denote by \( T_G \), which is a maximal connected abelian subgroup, and any two maximal algebraic tori in \( G \) are conjugate to one another. For \( GL(D) \), a canonical choice is the subgroup \( T(D) \) of invertible diagonal matrices, and for our \( G = GL(D_1) \times \cdots \times GL(D_m) \), a canonical choice is given by the subgroup \( T(D_1) \times \cdots \times T(D_m) \) consisting of all tuples of such matrices. Then, viewing \( \pi \) as a representation of \( T_G \), we may simultaneously diagonalise the action. The simultaneous eigenvalues are captured by the concept of weights of the representation:

**Definition V.6.** Let \( T_G \subseteq G \) be a maximal algebraic torus. Then there exists a unique finite set of weights \( \Omega(\pi) \subseteq Lie(T_G)^* \) of the representation \( \pi \), such that

\[
V = \bigoplus_{\omega \in \Omega(\pi)} V_{\omega}
\]

is an orthogonal decomposition into weight spaces \( V_{\omega} \), where

\[
\pi(e^Y) v_{\omega} = e^{\omega(Y)} v_{\omega}
\]

for all \( Y \in Lie(T_G) \) and \( v_{\omega} \in V_{\omega} \).

**Example V.7.** Let \( GL(D) \) act on \( Mat_{D \times D} \) by conjugation. As said before, a maximal subtorus of \( GL(D) \) is given by the set \( T(D) \) consisting of invertible diagonal \( D \times D \) matrices, and its Lie algebra \( Lie(T(D)) \) consists of all diagonal matrices, which may be identified with \( \mathbb{C}^D \). Then for \( Y \in \mathbb{C}^D \), we have

\[
e^{\text{diag}(Y)} E_{ij} e^{-\text{diag}(Y)} = e^{Y_{ij}} E_{ij},
\]

where \( E_{ij} \) are the elementary matrices. Therefore the weights are given by the functionals \( \omega_{ij}(Y) = Y_{ij} \), with corresponding weight spaces \( V_{\omega_{ij}} = \mathbb{C} E_{ij} \). Note that \( \omega_{ij} \) can be identified with \( \mathbb{C}^D \). The action of \( GL(D) \) on \( Mat_{D \times D} \) has the same weights, but now each weight space is \( d \)-dimensional.

Now consider the action of the gauge group \( G = GL(D_1) \times \cdots \times GL(D_m) \) on \( V = Mat_{D_1 \times \cdots \times D_m} \), the space of PEPS tensors, as defined in Definition IV.3. As mentioned, a maximal torus for \( G \) is given by \( T_G = T(D_1) \times \cdots \times T(D_m) \), and the Lie algebra of \( T_G \) may be identified with \( \mathbb{C}^{D_1} \oplus \cdots \oplus \mathbb{C}^{D_m} \). Then it is easy to show that the weights are just tuples of weights as above, i.e.,

\[
(e_{i_1} - e_{j_1}, \ldots, e_{i_m} - e_{j_m})
\]

with \( i_k, j_k \in [D_k] \) for \( k \in [m] \).

Given the general setting as above, we can now define the following two parameters:

**Definition V.8.** The weight margin \( \gamma(\pi) \) of the representation \( \pi \) is defined as

\[
\gamma(\pi) = \min\{d(0, \conv \Gamma) : \Gamma \subseteq \Omega(\pi), \ 0 \notin \conv \Gamma\}.
\]

Here, \( \conv \Gamma \) refers to the convex hull of \( \Gamma \subseteq Lie(T_G)^* \). The weight norm \( N(\pi) \) is defined by

\[
N(\pi) = \max\{\|\omega\|_2 : \omega \in \Omega(\pi)\}.
\]

The distance \( d(\cdot, \cdot) \) and \( \|\cdot\|_2 \) are defined in terms of the Hilbert-Schmidt inner product and identifying \( Lie(T_G)^* \equiv Lie(T_G) \subseteq Mat_{n \times n} \).

While these parameters are somewhat abstract, we give a short justification for their appearance being natural. As in Eq. (V.5), for a vector \( 0 \neq v \in V \) consider the function

\[
F_v(g) := \log\|g \cdot v\|_2.
\]

Considered as a function on the space of right cosets \( K \backslash G \), this is known as the Kempf-Ness function and it plays an important role in the general theory. Its gradient at the identity coset generalizes Eq. (V.6) and goes by the following name:

**Definition V.9.** The moment map \( \mu: V \setminus \{0\} \to \im Lie(K) \) is defined by

\[
\mu(v) = \nabla_{X=0} F_v(e^X) = \nabla_{X=0} \log\|e^X \cdot v\|_2.
\]

where \( X \in \im Lie(K) \).

This is also a moment map for the \( K \)-action on the projective space \( P(V) \) in the sense of symplectic geometry, which serves as a “collective Hamiltonian” for the action. If we restrict to the case where \( G \) is commutative, i.e., \( G = T_G \), then observe that for \( Y \in Lie(G) \) and \( v = \sum_{\omega \in \Omega(\pi)} v_{\omega} \) one has

\[
e^Y \cdot v = \sum_{\omega \in \Omega(\pi)} e^{\omega(Y)} v_{\omega},
\]

and since the decomposition into weight spaces is orthogonal, we get

\[
\|e^Y \cdot v\|_2^2 = \sum_{\omega \in \Omega(\pi)} e^{2\omega(Y)} \|v_{\omega}\|_2^2.
\]

From this expression, one can already see that if \( G \) is commutative, then \( F_v(e^Y) = \log\|e^Y \cdot v\|_2 \) is convex in \( Y \in \im Lie(K) \), and moreover that it is \( 2N(\pi)^2 \)-smooth. (This also holds for non-commutative \( G \), as can in fact be deduced from the preceding.) With the expression for \( \|e^Y \cdot v\|_2^2 \) we can compute the moment map by

\[
\mu(v)(Y) = \frac{\partial}{\partial t} \log\|\exp t Y \cdot v\|_2^2 = \frac{1}{\|v\|_2^2} \sum_{\omega \in \Omega(\pi)} \|v_{\omega}\|_2^2 \omega(Y),
\]

and we deduce that \( \mu(v) \) is a convex combination of the weights \( \omega \) for which \( v_{\omega} \neq 0 \). We observe now that the support \( \text{supp} v \),

\[
\text{supp} v \subseteq \{Y \in \im Lie(K) : \mu(v)(Y) \neq 0\}.
\]
For Theorem V.10 and Lemma V.11. We prove Theorem V.5, we still need to bound the parameters $\gamma(\pi)$ and $N(\pi)$ for our specific representations.

**Lemma V.11.** For the action of $G = \text{GL}(D_1) \times \cdots \times \text{GL}(D_m)$ on $V = \text{Mat}_{D_1 \times D_m}$, the weight norm $N(\pi)$ is given by

$$N(\pi) = \sqrt{2mn},$$

and the weight margin $\gamma(\pi)$ is lower bounded as

$$\gamma(\pi) \geq \gamma,$$

where $\gamma$ is the constant defined in Definition V.4.

**Proof.** The expression for the weight norm follows directly from Example V.7.

For $m = 1$, the lower bound on the weight margin follows from [52, Thm. 6.21]: the representation is a quiver representation, where the quiver is given by one vertex with $d$ self-loops. For $m \geq 2$, the lower bound on the weight margin follows from [52, Thm. 6.10].

**Proof of Theorem V.5.** This follows directly by combining Theorem V.10 and Lemma V.11.

Now that we know that Eqs. (V.2) and (V.3) can be related to each other, we will relate these to Eq. (V.1). In the one direction, it is clear that Eq. (V.1) implies a small error in the sense of Eq. (V.3):

$$\frac{\|S - T_{\text{min}}\|_2}{\|S\|_2} \leq \delta$$

implies

$$\frac{\|T_{\text{min}}\|_2}{\|S\|_2} \geq 1 - \frac{\|T_{\text{min}} - S\|_2}{\|S\|_2} = 1 - \delta$$

In the remainder of this section we show that Eq. (V.2) implies a small error in the sense of Eq. (V.1), closing the circle. It is useful to make the following abbreviation for Eq. (V.4), the gradient of the norm square function at the identity:

$$\tilde{\mu}(S) := \nabla f_S(I) = (\sigma_{k,1} - \sigma_{k,2})\sum_{k=1}^m$$

where $\sigma := |S\rangle \langle S|$, so $\tilde{\mu}(S) \in \text{Herm}(D_1) \oplus \cdots \oplus \text{Herm}(D_m)$.

We write $\tilde{\mu}$ and not $\mu$ to distinguish it from the gradient of the log-norm, as in Eq. (V.6) and Definition V.9, but note that

$$\|\tilde{\mu}(S)\|_2 = \varepsilon \text{tr}(\sigma) = \varepsilon \|S\|_2^2,$$

(V.7)

Then we will consider the gradient flow of $\|\tilde{\mu}(S)\|_2^2 := \sum_{k=1}^n \|\tilde{\mu}(S)\|_2^2$:

$$\frac{\text{d}}{\text{d}t} \|\tilde{\mu}(S)\|_2^2 = -\nabla \|\tilde{\mu}(S)\|_2^2$$

(V.8)

We will see that the solution $S(t)$ to this ODE remains in the gauge orbit of $S$ and that it converges to a minimal canonical form $S_{\text{min}}$ whose distance to $S$ in the sense of Eq. (V.1) can be controlled using Eq. (V.2).

The study of the gradient flow for the norm square of the moment map was pioneered in seminal work by Kirwan [94], and it found widespread use in mathematics. It was first proposed as an algorithmic tool in [49], [50] in the context of the quantum marginal problem, and analyzed quantitatively in [55] (to resolve the Paulsen problem) and [54] for the operator scaling action and then in [52] for general reductive group actions. While the following arguments work in complete generality, here we restrict to the gauge action of $G = \text{GL}(D_1) \times \cdots \times \text{GL}(D_m)$ since this is all we need.

We start by analyzing Eq. (V.8). Existence and uniqueness of the solution $S(t)$ of this ordinary differential equation on some maximal (possibly infinite) interval of definition $[0, t_{\text{max}})$, where $t_{\text{max}} \in [0, \infty)$, follows from Picard–Lindelöf theory. Then one can prove the following lemma, cf. [52, Prop. 3.27 and its proof]:

**Lemma V.12.** Let $S(t)$ be the solution to the dynamical system (V.8). Then, for all $t \in [0, t_{\text{max}})$, we have

1) $\frac{\partial}{\partial t} \frac{\|S(t)\|_2^2}{\|S\|_2^2} = -\frac{\|S(t)\|_2^2}{\|S\|_2^2}$
2) $\frac{\partial}{\partial t} \frac{\|S(t)\|_2^2}{\|S\|_2^2} = -8\|\tilde{\mu}(S(t))\|_2^2$
3) $S(t) \in G \cdot S$, i.e., the solution remains in the $G$-orbit of $S$ at all times.

**Proof.** The first claim holds for any gradient flow.

Next, we note that, for all $Y \in \text{Herm}(D_1) \oplus \cdots \oplus \text{Herm}(D_m)$,

$$\langle \tilde{\mu}(S), Y \rangle = \langle \nabla f_S(I) Y \rangle = \frac{1}{2} \sum_{k=0}^n \text{tr}(\{e^{Y_1}, \ldots, e^{Y_m}\} \cdot S)$$

(V.9)

where $X \cdot Y := \sum_{k=1}^m \text{tr}(X_k Y_k)$ and we denote by $\Pi(Y)$ the Lie algebra action of $Y$, which is defined by

$$\Pi(Y)S := \partial_{\varepsilon=0} (\{e^{\varepsilon Y_1}, \ldots, e^{\varepsilon Y_m}\} \cdot S).$$
By differentiating Eq. (V.9) with respect to $S$ in some direction $W \in V$ (an operation we denote by $D_W$),

$$
\langle D_W \tilde{\mu}(S), Y \rangle = \langle W, \Pi(Y)S \rangle + \langle S, \Pi(Y)W \rangle = 2 \operatorname{Re} \langle W, \Pi(Y)S \rangle.
$$

Accordingly, for all $W \in V$,

$$
D_W \|\tilde{\mu}(S)\|_2^2 = 2 \langle D_W \tilde{\mu}(S), \tilde{\mu}(S) \rangle = 4 \operatorname{Re} \langle W, \Pi(\tilde{\mu}(S))S \rangle.
$$

Thus we have proved that the gradient of $\|\tilde{\mu}\|_2^2$ is given by the following clean formula:

$$
\nabla \|\tilde{\mu}\|_2^2(S) = 4\Pi(\tilde{\mu}(S))S. \quad (V.10)
$$

The second item follows from this and Eq. (V.9),

$$
\partial_t \|S(t)\|_2^2 = 2 \langle S(t), S'(t) \rangle = -2 \langle S(t), \nabla \|\tilde{\mu}\|_2^2(S(t)) \rangle = -8 \langle S(t), \Pi(\tilde{\mu}(S(t)))S(t) \rangle = -8 \|\tilde{\mu}(S(t))\|_2^2.
$$

As Eq. (V.10) states that $S'(t)$ is a tangent vector of the $G$-orbit through $S(t)$, the third item also follows.

Using the preceding, the following key lemma shows that if $S_{\min} \neq 0$ then $\tilde{\mu}(S(t)) \to 0$ sufficiently quickly, without $S(t)$ moving too much. Our argument follows [55], which treats the case $m = 1$.

**Lemma V.13.** Let $S(t)$ denote the solution of Eq. (V.8) for a tensor $S(0) = S$ with $S_{\min} \neq 0$ (for some and hence for any minimal canonical form). Consider any $\tau$ such that $\tilde{\mu}(S(\tau)) \neq 0$. Then there exists

$$
\tau' \leq \tau + \frac{1}{4\gamma \|\tilde{\mu}(S(\tau))\|_2^2},
$$

such that

$$
\|\tilde{\mu}(S(\tau'))\|_2^2 = \frac{\|\tilde{\mu}(S(\tau))\|_2^2}{2}. \quad (V.11)
$$

(in fact $\tau'$ is the first time such that this is true) and, moreover,

$$
\|S(\tau') - S(\tau)\|_2 \leq \frac{1}{2\sqrt{2}} \sqrt{\frac{\|\tilde{\mu}(S(\tau))\|_2^2}{\gamma}}, \quad (V.12)
$$

where $\gamma$ is the constant from Definition V.4.

**Proof.** Suppose that $\tau' > \tau$ is such that

$$
\|\tilde{\mu}(S(\tau'))\|_2^2 > \frac{\|\tilde{\mu}(S(\tau))\|_2^2}{2}. \quad (V.13)
$$

By Item 1 of Lemma V.12,

$$
\|\tilde{\mu}(S(t))\|_2^2 > \frac{\|\tilde{\mu}(S(\tau))\|_2^2}{2} \quad \forall t \in [\tau, \tau']
$$

and hence, by Item 2 of the same lemma, for all $t \in [\tau, \tau']$

$$
\partial_t \|S(t)\|_2^2 = -8\|\tilde{\mu}(S(t))\|_2^2 < -4\|\tilde{\mu}(S(\tau))\|_2^2.
$$

Accordingly,

$$
\|S(\tau')\|_2^2 - \|S(\tau)\|_2^2 < 4(\tau' - \tau)\|\tilde{\mu}(S(\tau))\|_2^2.
$$

On the other hand, using the lower bound in Theorem V.5 and Eq. (V.7),

$$
\|S(\tau')\|_2^2 - \|S(\tau)\|_2^2 \geq \|S(\tau')_{\min}\|_2^2 - \|S(\tau)\|_2^2
\geq \|S(\tau)_{\min}\|_2^2 - \|S(\tau)\|_2^2
\geq \|S(\tau)\|_2^2 \left( \frac{\|S(\tau)_{\min}\|_2^2}{\|S(\tau)\|_2^2} - 1 \right)
\geq -\|\tilde{\mu}(S(\tau))\|_2^2.
$$

Together, we find that for any $\tau'$ such that Eq. (V.13) holds, we must have

$$
\tau' < \tau + \frac{1}{4\gamma \|\tilde{\mu}(S(\tau))\|_2^2}.
$$

Accordingly, there must exist some minimal

$$
\tau' \leq \tau + \frac{1}{4\gamma \|\tilde{\mu}(S(\tau))\|_2^2}, \quad (V.14)
$$

such that

$$
\|\tilde{\mu}(S(\tau'))\|_2^2 = \frac{\|\tilde{\mu}(S(\tau))\|_2^2}{2}. \quad (V.15)
$$

Moreover, for this $\tau'$ we have

$$
\|S(\tau') - S(\tau)\|_2 \leq \int_{\tau}^{\tau'} \|S'(t)\|_2 \, dt
\leq \int_{\tau}^{\tau'} \sqrt{-\partial_t \|\tilde{\mu}(S(t))\|_2^2} \, dt
\leq \sqrt{\int_{\tau}^{\tau'} \partial_t \|\tilde{\mu}(S(t))\|_2^2 \, dt} \sqrt{\int_{\tau}^{\tau'} \frac{1}{dt}}
\leq \sqrt{\frac{\|\tilde{\mu}(S(\tau))\|_2^2 - \|\tilde{\mu}(S(\tau'))\|_2^2}{\gamma}} \sqrt{\tau' - \tau}
\leq \frac{1}{2\sqrt{2}} \sqrt{\frac{\|\tilde{\mu}(S(\tau))\|_2^2}{\gamma}},
$$

where we used the triangle inequality, then Item 1 of Lemma V.12, then the Cauchy-Schwarz inequality, and finally Eqs. (V.14) and (V.15).

We now prove the desired relation between Eqs. (V.1) and (V.2):

**Theorem V.14.** Let $T$ be a tensor with $T_{\min} \neq 0$ (for some and hence for any minimal canonical form) and let $S \in G \cdot T$. Then there exists a minimal canonical form $T_{\min} \in G \cdot T$ such that

$$
\frac{\|S - T_{\min}\|_2}{\|S\|_2} \leq \sqrt{\frac{2\varepsilon}{\gamma}}
$$

for

$$
\varepsilon := \frac{1}{\operatorname{tr} \sigma} \sum_{k=1}^{m} \|\sigma_{k,1} - \sigma_{k,2}T\|_2^2.
$$

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where $\gamma$ is the constant from Definition V.4.

Proof. If $\mu(S) = 0$ then $T_{\min} = S$ is a minimal canonical form of $T$ and there is nothing to prove. Otherwise let us, for every $k \geq 0$, denote by $\tau_k$ the first time when
\[ \|\hat{\mu}(S(\tau_k))\|_2^2 \leq \frac{1}{2^k} \|\hat{\mu}(S)\|_2^2, \]
so $\tau_0 = 0$. By Lemma V.13,
\[ \tau_k = \sum_{i=1}^{k} (\tau_i - \tau_{i-1}) \leq \sum_{i=1}^{k} \frac{1}{4^i} \|\hat{\mu}(S(\tau_{i-1}))\|_2^2 = \frac{1}{4^k} \sum_{i=1}^{k} 1 \leq \frac{2^{k/2}}{\gamma \|\mu(S)\|_2}, \]
in particular, $\hat{\mu}(S(t)) \to 0$ as $t \to \infty$, since we know from Item 1 of Lemma V.12 that $\|\hat{\mu}(S(t))\|_2^2$ is monotonically decreasing.

Next, we prove that the subsequence $S(\tau_k)$ converges to a minimal canonical form of $T$ with the desired properties. We first show that the $S(\tau_k)$ form a Cauchy sequence. Indeed, for any $k \leq l$, using Lemma V.13,
\[ \|S(\tau_k) - S(\tau_l)\|_2 \leq \sum_{m=k+1}^{l} \|S(\tau_m) - S(\tau_{m-1})\|_2 \leq \sum_{m=k+1}^{l} \frac{1}{2^{2m-1}} \|\hat{\mu}(S(\tau_{m-1}))\|_2^2 \leq \frac{1}{\gamma} \|\hat{\mu}(S)\|_2^2 \sum_{m=k+1}^{l} \frac{1}{2^{2m-1}} \leq \frac{\sqrt{2} \|\hat{\mu}(S)\|_2}{\gamma} \leq \frac{\sqrt{2} \|\hat{\mu}(S)\|_2}{\gamma}, \]
which shows that indeed $S(\tau_k)$ is a Cauchy sequence. If we denote by $S'$ its limit, then $T' \in G \cdot S = G \cdot T$ (by Item 3 of Lemma V.12) and hence $T' \neq 0$ (since $T_{\min} \neq 0$ by assumption). Moreover, $\hat{\mu}(T') = 0$ by the above, hence $T'$ is a minimal canonical form of $T$. Finally,
\[ \|S - T\|_2 = \lim_{t \to \infty} \|S(\tau_0) - S(\tau_l)\|_2 \leq \frac{\sqrt{2} \|\hat{\mu}(S)\|_2}{\gamma} = \|S\|_2 \frac{\sqrt{2} \|\hat{\mu}(S)\|_2}{\gamma}, \]
using the preceding estimate and Eq. (V.7).

By combining Corollary V.3 and Theorem V.14 it follows that using the first-order algorithm in Algorithm 1 with $\varepsilon := \gamma \delta^2/2$ one can in time poly($\frac{1}{\gamma}, \frac{1}{\delta}$, input size) obtain a group element $g \in G$ such that the tensor $S := g \cdot T$ satisfies Eq. (V.1), i.e.,
\[ \|S - T_{\min}\|_2 \leq \delta. \]
In the next section we will see that the dependence on $\delta$ can be improved to $\log(1/\delta)$, see Corollary V.16.

C. Second-order algorithm

As promised earlier, there is also a second numerical method that one can use to approximate normal forms in our setting. This is a more sophisticated second-order method, which uses information about the Hessian of the Kempf–Ness function $F_v$ to determine the direction in which to move (as is done for instance in Newton’s method), whereas the first-order method discussed in Section V-A and Algorithm 1 before only use information about the gradient.

In [52, Algo. 5.2], a “box-constrained Newton method” is analyzed, which uses Newton steps constrained to a constant-sized box to make progress in the objective. It naturally minimizes the norm of the resulting vector (as opposed to the size of the gradient). Its guarantees applied to our setting are as follows:

**Theorem V.15** ([52, Thm. 8.12]). Let $T$ be a tensor in $\text{Mat}_{D_1 \times \ldots \times D_m}$ such that $T_{\min} \neq 0$ (for some and hence for any minimal canonical form). Assume that the entries of $T$ are in $\mathbb{Q}[i]$ and given by storing the numerators and denominators in binary. Then there exists an algorithm that, given $T$ and $0 < \delta < 1$, returns a group element $g \in \text{GL}(D_1) \times \ldots \times \text{GL}(D_m)$ such that the tensor $S := g \cdot T$ satisfies $\|S\|_2 \leq \|T\|_2$ and
\[ \log \frac{\|S\|_2}{\|T\|_2} \leq \zeta \quad \text{and hence} \quad \frac{\|T_{\min}\|_2}{\|S\|_2} \geq 1 - \zeta \]
in time poly$(\gamma^{-1}, D_1, \ldots, D_m, \log(1/\zeta), \langle T \rangle)$, where $\gamma$ is defined in Definition V.4, and $\langle T \rangle$ is the total number of bits used to represent $T$.

By combining Theorem V.15 with the results of Section V-B, we arrive at the following result which was stated informally as Result 4 in the introduction.

**Corollary V.16.** Let $T \in \text{Mat}_{D_1 \times \ldots \times D_m}^{d_1 \times \ldots \times d_m}$ be a tensor such that $T_{\min} \neq 0$ (for some and hence for any minimal canonical form). Assume that the entries of $T$ are in $\mathbb{Q}[i]$ and given by storing the numerators and denominators in binary. Then there exists an algorithm that, given $T$ and $0 < \delta < 1$, returns a group element $g \in \text{GL}(D_1) \times \ldots \times \text{GL}(D_m)$ such that the tensor $S := g \cdot T$ satisfies $\|S\|_2 \leq \|T\|_2$ and
\[ \|S - T_{\min}\|_2 \leq \delta, \]
in time poly$(\gamma^{-1}, D_1, \ldots, D_m, \log(1/\delta), \langle T \rangle)$, where $\gamma$ is defined in Definition V.4, and $\langle T \rangle$ is the total number of bits used to represent $T$.

Proof. Apply the algorithm of Theorem V.15 with
\[ \zeta := \frac{\gamma^2}{64m} \delta^4 \quad \text{(V.16)} \]
to obtain in the stated runtime a group element $g \in G$ such that the tensor $S := g \cdot T$ satisfies $\|S\|_2 \leq \|T\|_2$ and
\[ \frac{\|T_{\min}\|_2}{\|S\|_2} \geq 1 - \zeta \quad \text{and hence} \quad \frac{\|T_{\min}\|_2^2}{\|S\|_2^2} \geq 1 - 2\zeta. \quad \text{(V.17)} \]
We now check that $S$ satisfies the desired condition. First, by Theorem V.5, for $\sigma = |S\rangle \langle S|$ we have that
\[ \frac{\|T_{\text{min}}\|^2}{\|S\|^2} \leq 1 - \frac{\varepsilon^2}{8m} \]
for
\[ \varepsilon := \frac{1}{8m} \sum_{k=1}^m \|\sigma_{k,1} - \sigma_{k,2}\|^2, \]
and hence, using Eq. (V.17),
\[ \varepsilon \leq \sqrt{8m \left( 1 - \frac{\|T_{\text{min}}\|^2}{\|S\|^2} \right)} \leq 4\sqrt{m\zeta}, \quad \text{(V.18)} \]
Finally, Theorem V.14 implies that
\[ \frac{\|S - T_{\text{min}}\|}{\|S\|} \leq \sqrt{\frac{2\varepsilon}{\gamma}} \]
and hence
\[ \frac{\|S - T_{\text{min}}\|}{\|S\|} \leq \sqrt{\frac{2\varepsilon}{\gamma}} \leq \sqrt{\frac{8\sqrt{m\zeta}}{\gamma}} \leq \delta, \]
where used Eq. (V.18) and our choice of $\zeta$ in Eq. (V.16). This concludes the proof. \(\square\)

**Remark V.17.** While Corollary V.16 uses relative $\ell^2$-error, which is most natural, we can also obtain a guarantee in absolute error, say
\[ \|S - T_{\text{min}}\| \leq \delta', \]
by applying Corollary V.16 with $\delta < \min(1, \delta'/\|T\|)$. As the second-order algorithm scales polynomially in $\log(1/\delta)$, this still runs in time $\text{poly}(\gamma^{-1}, D_1, \ldots, D_m, \log(1/\delta'), \langle T\rangle)$.

**VI. Conclusion and Outlook**

The current work is a theoretical one, proposing a new canonical form and proving some of its key properties. The fact that the minimal canonical form is rigorous in the sense that it can be proven to always exist as well as satisfy the basic properties discussed in Section IV sets it apart from other heuristic approaches [32], [35]. Besides this, we hope that the minimal canonical form will be of practical use in tensor network algorithms. Below we outline four potential directions for application. Detailed numerical study will be required to confirm the usefulness of these suggestions.

1) **Truncation of bond dimensions.** In many tensor network algorithms truncation of the bond dimension is a crucial step. This is especially the case for ground state finding algorithms based on imaginary time evolution (Time Evolving Block Decimation, TEBD) in which each step consist of applying an operator to the tensor network which increases the ground state approximation accuracy but also the bond dimension, and then truncating the bond dimension. One is given a tensor $T$ with a certain bond dimension $D$, and one would like to find a tensor $T'$ with a prescribed bond dimension $D' < D$ such that the tensor network state using $T$ is approximated as accurately as possible by the tensor network state using $T'$. In one spatial dimension, for MPS, there is a natural way to do this using canonical forms. For instance, one may use the left canonical form, in which case the reduced state $\rho_2$ on the right virtual dimension is maximally mixed. Then one truncates to the subspace spanned by the eigenvectors of the $D'$ largest eigenvalues of the reduced state $\rho_1$ on the left virtual dimension.

The bond dimension truncation scheme for MPS is both computationally efficient and gives an optimal approximation given a prescribed bond dimension. For two-dimensional PEPS there is no truncation scheme known which has both these desirable properties, which is closely related to the lacking of the equivalent of a left or right canonical form. Various methods exist [34], [95], see for instance [37] for an overview of different methods. While these methods perform well in practice, in most cases good theoretical understanding is lacking. Here, we propose the following natural truncation scheme: given a tensor $T$, compute its minimal canonical form $S$. Then truncate to the subspace spanned by the eigenvectors corresponding to the $D'$ largest eigenvalues.

This proposal leads various questions which should be addressed in follow-up work. First of all, it would be interesting to use such a truncation method in existing PEPS algorithms and study the performance of such schemes numerically. Secondly, as our methods are designed for uniform (translation-invariant) systems one would hope that they are also of use to iPEPS methods, where precisely the absence of a canonical form has led to heuristic approaches to gauge-fixing [35], [36] which work well in practice. We would like to emphasize that especially the (non-rigorously defined) canonical form in [35] is fairly close in spirit to the minimal canonical form: it is defined by a condition similar (but different) to the characterization in Theorem IV.8. This canonical form has been shown to indeed improve convergence of imaginary time evolution algorithms, which offers some hope for the prospect of using the minimal canonical form for truncation purposes. Finally, a potential advantage of truncation schemes based on the minimal canonical form is that one could attempt to the framework of geometric invariant theory to prove that such a truncation scheme has good theoretical properties.

2) **Numerical stability.** Using minimal canonical forms in variational algorithms may be helpful, since appropriate gauge fixing is known to enhance the stability of variational algorithms [36], [66].

3) **Boundary-based approaches.** PEPS have a very useful and explicit bulk-boundary correspondence [79], which allows one to map bulk properties in a region $R$ to properties of the associated boundary state $\rho_{\text{B}}$, defined essentially as the reduced density matrix in the virtual indices of the PEPS tensor $|T_R\rangle$ obtained after blocking
the original PEPS tensor $T$ in the given region $R$. The key insight of [79], formalized later in [96], [97], is that if one interprets $\rho_R$ as a Gibbs state $\rho_R = e^{-H_E},$ the properties of $H_E$ (the so-called entanglement Hamiltonian) encode the properties of the bulk of the system. This has led for instance to new numerical methods to detect topological phase transitions [98]. Since $H_E$ and $\rho_R$ live in the virtual Hilbert space, it is crucial for this approach to be meaningful that the only gauge freedom one considers comes from unitaries, which do not change any of the relevant properties of $H_E$ or $\rho_R,$ rather than arbitrary invertible matrices. This is precisely what is ensured by working with the minimal canonical form.

4) **Privacy in PEPS-based machine learning algorithms.** Tensor networks, and PEPS and MPS in particular, have been used as variational Ansätze in machine learning contexts [19], [20]. This has the appeal that one can import known optimization techniques in condensed matter problems to machine learning. Another potential advantage, compared to neural network-based approaches, lies in a higher interpretability; it is precisely the characterization of global properties in the local tensors of a tensor network which explains its success in quantum many-body problems. In [67] a new potential advantage of tensor networks in a machine learning context has been proposed, which we will now explain briefly. There are two possible ways to look at a trained neural network or tensor network: as a black box in which one has only access to the input-output relation or as a white box in which all internal parameters are provided. It is shown in [67], with machines trained in real data bases with medical records, that those internal parameters can reveal sensitive information from the training data set which however are not contained in the black-box picture. This white-box versus black-box scenario is the underlying problem behind obfuscation protocols⁹ and it is well known there that the perfect solution comes from the existence of a well-defined canonical form for the white-boxes that maps them one-to-one to the set of black boxes. The basic idea in [67] is that this can be done in MPS by defining a new canonical form which selects analytically and uniquely an element for each orbit of a normal MPS. However, as it is also discussed in [67], a way of sampling uniformly on all possible white-box representations of the same black-box function could equally do the job.

The minimal canonical form gives a way to extend this idea trivially to general PEPS. If the presentation (white-box) of the PEPS obtained in the training process is its minimal canonical form, sampling uniformly on all possible white-boxes amounts to sampling with the Haar measure on the unitary group, which can easily be done (as opposed to sampling on the whole general linear group). It is an interesting open question to see how this idea works in practice for PEPS. For MPS it is shown in [67] that privacy improvements in practice are indeed dramatic.

As alluded to in Section IV-D another natural direction of inquiry is to find physically relevant models where there is topological order which is only revealed on manifolds other than a torus, and see how this relates to the minimal canonical form. Finally, it would be interesting to connect to recent approaches that apply techniques from algebraic geometry and algebraic complexity theory [99] to tensor network theory, for instance [100]–[102]. There are also various concrete follow-up questions concerning properties of the minimal canonical form and generalizations.

1) **Non-uniform PEPS** In this work we have mainly restricted to uniform PEPS, where we consider contractions of copies of a single identical tensor. We also saw one example with non-uniform tensors, for MPS in Section III-C. In that case, we were able to recover the usual theory of canonical forms for MPS with open boundary conditions. Clearly, an interesting direction for future research is to investigate generalizations of the minimal canonical form to non-uniform PEPS. In this case we consider a fixed graph $\Gamma = (V,E)$, with a collection of tensors $(T_v)_{v \in V}$ at each vertex and where we contract along the edges $E$. We now have a group $GL(D_e)$ acting on each edge $e$ in the graph, so the full gauge group $G$ is the product over all edges $e \in E$ of these groups. This setup is very similar to the one described in Section III-C. We would like to formulate an appropriate minimization problem over a group orbit. There are two obvious ways to approach this. The first option is to minimize

$$\sum_{v \in V} \| g \cdot f_v \|_2^2$$

and define a minimal canonical form $((T_v)_{v \in V})_{\text{min}}$ by

$$\text{arg min} \left\{ \sum_{v \in V} \| S_v \|_2^2 : (S_v)_{v \in V} \in \mathcal{G} \cdot (T_v)_{v \in V} \right\}.$$

In the case where all tensors are equal, this should reduce to the minimal canonical form for uniform PEPS. A second option (which is similar to the MPS construction in Section III-C) would be to consider for each edge $e$ the tensor network state $|T_e \rangle$ where we have contracted all edges except $e$. We have a group action of $GL(D_e)$ on this state, and we may minimize over its orbit. We will report on these generalizations in future work.

2) **Algorithms for deciding gauge equivalence** While we have addressed the issue of computing a minimal canonical form for a given tensor, we have not extensively discussed algorithms for deciding whether two tensors $S$ and $T$ are gauge equivalent. One approach is given by Result 3: one may simply check that $|S_\pi \rangle = |T_\pi \rangle$ for all $\pi \in S_n^m$ with $n \leq n_{\text{max}} = \exp(O(m^2D^2 \log(mD)))$ (or in the case of MPS, for $n \leq 2^D$). However, an alternative strategy is as follows. By Theorem IV.7, it suffices to first compute minimal canonical forms $S_{\text{min}}$ and $T_{\text{min}}$ (for which we

⁹Though the inherent continuous nature of the variables makes the problem slightly different in this case.
have already provided algorithms) and then determine whether these are related by unitary gauge transformations (which is rather nontrivial). For \( n = 1 \), this strategy has been implemented in [54], while for \( n \geq 2 \) we defer to future work.

3) Computational complexity. It would be interesting to relate the computation of minimal canonical forms and of checking gauge equivalence to other orbit problems that have recently been studied intensely in the theoretical computer science literature, in order to get a better understanding of the computational complexity of the problem (see [52] and references therein).

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