Tensor Network Methods in Many-body physics

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Abstract

Strongly correlated systems exhibit phenomena – such as high-T_C superconductivity or the fractional quantum Hall effect – that are not explicable by classical and semi-classical methods. Moreover, due to the exponential scaling of the associated Hilbert space, solving the proposed model Hamiltonians by brute-force numerical methods is bound to fail. Thus, it is important to develop novel numerical and analytical methods that can explain the physics in this regime.

Tensor Network states are quantum many-body states that help to overcome some of these difficulties by defining a family of states that depend only on a small number of parameters. Their use is twofold: they are used as variational ansatzes in numerical algorithms as well as providing a framework to represent a large class of exactly solvable models that are believed to represent all possible phases of matter. The present thesis investigates mathematical properties of these states thus deepening the understanding of how and why Tensor Networks are suitable for the description of quantum many-body systems.

It is believed that tensor networks can represent ground states of local Hamiltonians, but how good is this representation? This question is of fundamental importance as variational algorithms based on tensor networks can only perform well if any ground state can be approximated efficiently in such a way. While any state can be written as a tensor network state, the number of parameters needed for the description might be too large. This is not the case for one-dimensional systems: only a few parameters are required to have a good approximation of their ground states; that, in turn, allows for numerical algorithms based on tensor networks performing well. The situation in two dimensions is somewhat more complicated, but it is known that ground states of local Hamiltonians can be expressed as tensor networks with sub-exponentially many parameters. In the present thesis, we improve on these existing bounds strengthening the claim that the language of tensor networks is suitable to describe many-body systems.

Another central question is how symmetries of the system such as translational invariance, time-reversal symmetry or local unitary symmetry can be reflected in tensor networks. This question is important as systems appearing in nature might intrinsically possess certain symmetries; on one hand, understanding these symmetries simplifies the description of these systems. On the other hand, the presence of symmetries leads to the appearance of novel phases – symmetry-protected topological (SPT) order, – and tensor networks provide the right language to classify these phases. In one dimension and for

certain classes of two-dimensional tensor networks (states generated by so-called injective tensors) it is well understood how symmetries of the state can be described. A general framework, however, has yet to be developed. In the present thesis, we contribute to the development of the theory in two ways. We first investigate the question for injective tensors, and generalize the existing proof for any geometry including the hyperbolic geometry used in the AdS/CFT correspondence. Second, we introduce a class of tensor network states that include previously known examples of states exhibiting SPT order. We show how symmetries are reflected in these states thus deepening the understanding of SPT order in two dimensions.

Zusammenfassung

Stark korrelierte Systeme zeigen Phänomene wie Hochtemperatursupraleitung oder den Quanten-Hall-Effekt, die mit klassischen und semiklassischen Methoden nicht erklärbar sind. Da die Dimension des zugrundeliegenden Hilbertraums exponentiell mit der Größe des Systems wächst, versagen viele der traditionellen Ansätze für derartige Systeme. Es ist daher notwendig, neuartige numerische und analytische Methoden zu entwickeln, die die Physik in diesem Bereich erklären können.

Tensor-Netzwerkzustände können diese Schwierigkeiten zum Teil überwinden, indem sie eine Familie von Zuständen definieren, die nur von einer kleinen Anzahl von Parametern abhängen. Diese Zustände tragen auf zwei Arten zur Lösung des Problems bei: Erstens werden sie als Variationsansatz in numerischen Algorithmen verwendet. Zweitens bieten sie einen analytischen Zugang zu einer großen Klasse genau lösbarer Modelle, von denen angenommen wird, dass sie alle möglichen Materiephasen repräsentieren. In der vorliegenden Arbeit werden mathematische Eigenschaften dieser Zustände untersucht, wodurch das Verständnis dafür, wie und warum Tensor-Netzwerke für die Beschreibung von Quantensystemen geeignet sind, vertieft wird.

Zunächst widmen wir uns der Frage, inwiefern Tensornetzwerke Grundzustände lokaler Hamiltonians darstellen können. Diese Frage ist von grundlegender Bedeutung, da Variationsalgorithmen, die auf Tensornetzwerken basieren, nur dann akkurate Ergebnisse liefern können, wenn der Grundzustand nicht allzu weit von der zugrundeliegenden variationellen Mannigfaltigkeit entfernt ist. Zwar kann prinzipiell jeder Quantenzustand als Tensornetzwerkstatus beschrieben werden. Jedoch ist die Anzahl der für die Beschreibung erforderlichen Parameter möglicherweise extrem groß. Dies ist bei eindimensionalen Systemen nicht der Fall: Nur wenige Parameter sind erforderlich, um eine gute Näherung ihrer Grundzustände zu erhalten. Aufgrund dieser theoretische Grundlage kann darauf vertraut werden, dass die Ergebnisse der tensornetzwerkbasierten Algorithmen akkurat sind. Die Situation in zwei Dimensionen ist komplizierter, aber es ist bekannt, dass Grundzustände lokaler Hamiltonians als Tensornetzwerke mit subexponentiell vielen Parametern ausgedrückt werden können. In der vorliegenden Arbeit verbessern wir diese bestehenden Grenzen und verstärken die Behauptung, dass Tensornetzwerke geeignet ist, Vielteilchensysteme zu beschreiben.

Eine weitere zentrale Frage ist, wie Symmetrien des Systems wie Translationsinvarianz, Zeitumkehrsymmetrie oder lokale Symmetrie in Tensornetzwerken reflektiert werden können. Das Verständnis dieser Symmetrien vereinfacht einerseits die Beschreibung der

Systeme, in denen diese Symmetrien auftreten. Auf der anderen Seite führt das Vorhandensein von Symmetrien zum Entstehen neuer Phasen - sogenannter “symmetry protected topological phases” (SPT) -, und Tensornetzwerke liefern die richtige Beschreibung, um diese Phasen zu klassifizieren. In einer Dimension und für bestimmte Klassen von zweidimensionalen Tensornetzwerken (Zustände, die von sogenannten injektiven Tensoren erzeugt werden) ist es gut verstanden, wie Symmetrien des physikalischen System sich in ihrer Beschreibung als Tensornetzwerk widerspiegeln. Ein allgemeiner Rahmen muss jedoch noch entwickelt werden. In der vorliegenden Arbeit tragen wir auf zweierlei Weise zur Weiterentwicklung der Theorie bei. Wir untersuchen zunächst die Frage nach injektiven Tensoren und verallgemeinern den vorhandenen Beweis für jede Geometrie, einschließlich der in der AdS / CFT-Korrespondenz verwendeten hyperbolischen Geometrie. Zweitens führen wir eine Klasse von Tensornetzwerkzuständen ein, die bereits bekannte Beispiele für Zustände mit SPT-Ordnung enthalten. Wir zeigen, wie sich Symmetrien in diesen Zuständen widerspiegeln, wodurch das Verständnis der SPT-Ordnung in zwei Dimensionen vertieft wird.

List of publications

First author publications:

1. Andras Molnar, Norbert Schuch, Frank Verstraete, and J. Ignacio Cirac. "Approximating Gibbs states of local Hamiltonians efficiently with projected entangled pair states". In: *Phys. Rev. B* 91.4, 045138 (4 Jan. 2015), p. 045138. arXiv: 1406.2973

2. Andras Molnar, Yimin Ge, Norbert Schuch, and J. Ignacio Cirac. "A generalization of the injectivity condition for Projected Entangled Pair States". In: *J. Math. Phys. 59, 021902 (2018)* 59.2, 021902 (June 22, 2017), p. 021902. arXiv: 1706.07329v1

3. Andras Molnar, José Garre-Rubio, David Pérez- García, Norbert Schuch, and J. Ignacio Cirac. "Normal projected entangled pair states generating the same state". In: *New J. Phys.* 20, 113017 (Nov. 2018), p. 113017. arXiv: 1804.04964

Non-first author publications:

1. Yimin Ge, András Molnár, and J. Ignacio Cirac. "Rapid Adiabatic Preparation of Injective Projected Entangled Pair States and Gibbs States". In: *Phys. Rev. Lett.* 116.8 (Feb. 2016), arXiv:1508.00570. arXiv: 1508.00570

2. Ilya Kull, Andras Molnar, Erez Zohar, and J. Ignacio Cirac. "Classification of Matrix Product States with a Local (Gauge) Symmetry". In: *Annals of Physics, Volume 386, November 2017, Pages 199-241* 386 (Aug. 1, 2017), pp. 199–241. arXiv: 1708.00362v2

3. G. Scarpa et al. "Computational complexity of PEPS zero testing". In: *ArXiv e-prints* (Feb. 22, 2018). arXiv: 1802.08214

4. David Sauerwein, Andras Molnar, J. Ignacio Cirac, and Barbara Kraus. "Matrix Product States: Entanglement, symmetries, and state transformations". In: *arXiv e-prints*, arXiv:1901.07448 (Jan. 2019), arXiv:1901.07448. arXiv: 1901.07448

Contents

Chapter 1

Introduction

Condensed matter physics tries to explain how macroscopic properties of materials arise from their microscopic structures. This understanding can be used to engineer new materials such as superconductors withstanding high magnetic fields or temperatures, or semiconductors used in modern electronics. Microscopic models in condensed matter are however very hard to solve, due to the exponential scaling of parameters with the number of particles. Despite this theoretical difficulty, the macroscopic properties of many systems can be explained as a single particle interacting with an effective environment composed of the other particles, which makes the understanding of these systems relatively easy. For some physical phenomena, however this mean-field approach fails due to the presence of strong correlations. Examples of such phenomena include high-T_C superconductivity [8, 9], the fractional quantum Hall effect [10] and topological insulators.

The bottleneck in the understanding of materials consists in solving the proposed first-principle models; therefore, simplified, effective Hamiltonians are often introduced. These effective models, despite their simplified form, are expected to capture the relevant physics, in particular the low-energy behavior of the system. Some prominent examples are the Hubbard model which is expected to capture essential physics of high-T_c superconductivity, or the Heisenberg model proposed to explain (quantum) magnetism[1]. Due to the crystal structure of solids, effective models are often defined on a lattice; that is, the positions of the particles are fixed at the vertices of a lattice and the model is defined on some internal degrees of freedom of the particles. The interaction is often restricted to be local, for example to nearest-neighbor interactions. In case of the Heisenberg model, the internal degree of freedom of the particles is their spin, while their positions are, for example, fixed on a one- or two-dimensional square lattice. Their interaction is described by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j, \tag{1.1}$$

where J is the strength of the interaction, $\mathbf{S}_i$ is the spin operator acting on the spin at position i, and the summation is restricted to neighboring positions. Apart from these

[1] The antiferromagnetic Heisenberg model is in fact the large U/t limit of the Hubbard model.

effective models, lattice models also arise as discretized versions of first-principle models such as in quantum chemistry or in lattice gauge theory.

Despite the simplicity of effective models, solving them (that is, obtaining the ground state and low energy excitations or the Gibbs state) remains challenging. The reason is that the Hilbert space used to describe the state of the system grows exponentially with the number of particles, therefore not only finding a solution, but already describing it is very hard for large system sizes. For example, describing and storing a state of 100 particles with only two degrees of freedom (qubits) is already impossible. There are a number of ways around this "curse of dimensionality" [11] such as Quantum Monte Carlo methods, variational methods, creation of exactly solvable models or quantum simulation.

Quantum Monte Carlo methods [12] build on the observation that the physically interesting quantity is not the wave function itself, but rather expectation values (and correlations) of local observables. This observation leads to sampling techniques adapted from classical stochastic modeling. While such techniques are very effective in many situations, they often suffer from the infamous sign problem making them inadequate to simulate fermions and frustrated systems.

In variational methods, one considers a set of states that are easy to store and to calculate with, and tries to find the minimum-energy state amongst them. Obviously, this method can lead to false results if the variational ansatz does not contain states from the low-energy sector of the Hamiltonian. An example for such a variational ansatz is the set of product states in the Hartree method (mean-field theory), or the use of Slater determinants in the Hartree-Fock method [13]. The latter is widely used in quantum chemistry.

The idea behind creating exactly solvable models is the following. In certain situations such as in frustrated spin systems, obtaining information about the model is very hard. One still wants to understand how global responses emerge from the microscopic description of the model. Exactly solvable models lead to such an insight by providing models with complete understanding. This, in fact, can indicate how real world models can behave and what are the important aspects of the different models.

In quantum simulation, a well-controlled quantum system is constructed to simulate the model. Such quantum systems can either serve as fully-fledged quantum computers, or as systems where despite the lack of control over every degree of freedom, some parameters can be adjusted in a way such that the system is governed by the Hamiltonian under investigation. While experimental realization of fully-fledged quantum computers is still far away, cold atoms in optical lattices [14] and trapped ions in RF traps [15] provide enough control already in current experiments for modeling interesting Hamiltonians.

In the present thesis, we investigate properties of Tensor Network States (TNS) [16] that can be thought of both as a variational ansatz for many-body Hamiltonians and as a language for creating and analyzing exactly solvable models. Tensor Network states include the one-dimensional Matrix Product States (MPS) [17, 18] ansatz, their higher dimensional generalization, Projected Entangled Pair States (PEPS) [19, 20], and the Multi-scale Renormalization Ansatz (MERA) [21] reflecting the scale invariance of critical systems. Algorithms based on MPS are extremely successful in approximating ground states of one-dimensional many-body systems. In two dimensions, algorithms based on

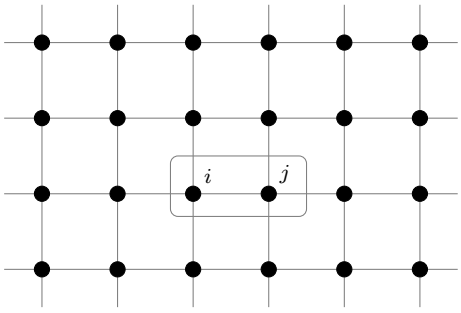
PEPS are more difficult to implement but have been gaining popularity in recent years. But is it theoretically justified to use PEPS as a variational ansatz? We investigate this question and improve on already existing results on how well PEPS can approximate ground states of local Hamiltonians. Due to their success in describing relevant physics, it is believed that a classification of Tensor Networks (TNs) provides us with a classification of phases. In one dimension, this has been carried out with the help of MPS, both in the presence and absence of symmetries [22, 23]. To arrive at this classification, it was necessary to understand how symmetries of the state can be reflected in the corresponding tensor networks.

In two dimensions, TNs are known to be able to represent certain topologically ordered phases. This means that for certain types of topological quantum field theories (TQFTs), they provide examples of local Hamiltonians realizing the corresponding topological order. In the presence of symmetries, they can be used to construct examples for symmetry-enriched (SET) and symmetry-protected topological (SPT) phases. In the understanding of these models, it is crucial to know how symmetries are reflected in the generating tensors. It is, however, only known for concrete examples and a special class of tensors known as injective or normal tensors. We broaden the understanding of how symmetries are represented in TNS by developing new methods for deciding whether two given tensors generate the same states or not.

1.1 Spin lattice models

Before introducing Tensor Networks, let us briefly recall what spin lattice models are and what "solving" such a model means. Apart from that, we give a mathematical definition of gapped phases, and show how some of their expected properties follow from the definition. We also recall when a phase is called topologically ordered (both intrinsic and symmetry-protected).

Let us consider spins arranged on a lattice (for example, a line in one dimension, or square lattice or Kagome lattice in two dimensions). The joint state of N such d-dimensional particles is described on the Hilbert space $(\mathbb{C}^d)^{\otimes N}$. We consider models where the interaction of the particles is geometrically local, i.e. local Hamiltonians such as nearest-neighbor Hamiltonians:



$$H = \sum_{\langle i,j \rangle} h_{ij},$$

where i and j label lattice sites and the sum runs over all pairs that are connected with an edge. The term h_{ij} is acting non-trivially only on the particles i and j, that is, h_{ij} has

the following form:

$$h_{ij} = \bigotimes_{k \notin \{i,j\}} \mathrm{Id}_k \otimes \tilde{h}_{ij},$$

where $\tilde{h}_{ij}$ is a two-body operator.

The Hamiltonian, apart from determining the dynamics, defines the state of the system ρ in equilibrium, as described below. Once the state of the system is known, expectation values of (local) observables can be calculated as well as their (connected) correlation functions:

$$\begin{aligned} \langle O \rangle &= \mathrm{Tr}\{O\rho\} \\ \mathrm{Corr}(O_i, O_j) &= \langle O_i O_j \rangle - \langle O_i \rangle \cdot \langle O_j \rangle, \end{aligned}$$

where O_i is the local operator O acting on the i^{th} particle:

$$O_i = \bigotimes_{k \neq i} Id_k \otimes O.$$

Correlation functions such as spin-spin correlations can be measured through scattering experiments and can thus be used to obtain information about the Hamiltonian.

The state ρ describing the system is defined by the Hamiltonian in the following way. Due to for example, electromagnetic radiation, the system is never perfectly isolated and thus perturbations are always present. Due to the perturbations, the state of the system always changes, and instead of trying to completely determine it, a statistical description is used. That is, one assigns a density matrix (classically, a probability distribution) to it that gives back the average expectation values of observables. The way to assign this density matrix is via the principle of maximum uncertainty. That is, the guessed density matrix (probability distribution) is the one that contains the least information on the system: the maximum entropy state. In thermal equilibrium, however, there is an extra information known: the energy is constant. Therefore the system is described by the maximum entropy state such that the energy E is fixed:

$$\hat{\rho} = \underset{\mathrm{Tr}\{\rho H\} = E}{\mathrm{argmin}} \; S(\rho),$$

where $S(\rho) = -\operatorname{Tr} \rho \log \rho$ is the von Neumann entropy. The solution of this minimization is the Gibbs state:

$$\rho = \frac{e^{-\beta H}}{Z} = \frac{e^{-\beta H}}{\operatorname{Tr}\left[e^{-\beta H}\right]}, \tag{1.2}$$

where Z is the partition function and $\beta = 1/k_B T$ is the inverse temperature. At zero temperature $\beta \to \infty$, and the system is in the lowest-energy state $|\Psi\rangle$ (ground state) of the Hamiltonian:

$$\rho = \lim_{\beta \to \infty} \frac{e^{-\beta H}}{Z} = |\Psi\rangle\langle\Psi|.$$

If the ground state is separated from the rest of the spectrum by a spectral gap and the density of states does not scale too badly with the energy and the system size N ($\Omega(E) \leq e^{\gamma NE}$), then the system is in the ground state already for an inverse temperature that grows only logarithmically with the system size, i.e. $\beta \propto \log N$. The logarithmic scaling is essential in providing a usable bound: macroscopic systems contain $\sim 10^{23}$ particles, thus linear scaling would result in a bound on the temperature that is practically indistinguishable form zero.

The presence or absence of the spectral gap has other, far-reaching consequences. For example, for a Hamiltonian that describes electrons moving in a material, it reveals whether the model describes a conductor or insulator: if the Hamiltonian is not gapped, then even a small electric field creates excitations and hence the material is a conductor. On the other hand, if a spectral gap is present, then the material is an insulator or semiconductor. Another property that is governed by the spectral gap is the behavior of heat capacity at low temperatures. If a spectral gap is present, then the heat capacity disappears as an exponential of the inverse temperature, and otherwise the heat capacity has a power-low behavior in the inverse temperature.

Even though it is intuitive physically what spectral gap means, mathematically it is a bit more involved to describe. It can either be defined directly in the thermodynamic limit, or, probably a bit simpler, by considering a family of models with larger and larger system sizes approaching the TD limit. We follow this second approach. Let H_n be a family of Hamiltonians on increasing system sizes. Let $\Delta_n = E_n^1 - E_n^0$ be the energy gap between the first excited state and the ground state energy of H_n. The model associated with the family of Hamiltonians H_n is called gapped if $\Delta_n \geq \Delta$ for any large enough n and some constant $\Delta > 0$.

Given the definition above, it can be proven that correlations in a gapped system decay exponentially [24]. The key tool in the proof is the Lieb-Robinson bound and it is interesting on its own. It states that perturbations in a local spin lattice model travel with finite speed, i.e. for any local operator A and B,

$$\big|[B(t), A(0)]\big| \leq \|A\| \cdot \|B\| \cdot e^{-\mu d_{AB}} \cdot (e^{vt} - 1),$$

where μ and v are some positive constants, d_{AB} is the distance of the sites on which the operators act and $B(t) = e^{iHt}Be^{-iHt}$. This can indeed be interpreted as perturbations propagating at a speed v: the operator A detects the perturbation B only after a time proportional to $t = d_{AB}/v$.

In case of a unique ground state, the decay of the correlations holds for the connected correlation functions. If the Hamiltonian has degenerate ground states, then the quantity that decays exponentially is

$$\langle\Psi|O_iO_j|\Psi\rangle - \frac{1}{2}(\langle\Psi|O_iPO_j|\Psi\rangle + \langle\Psi|O_jPO_i|\Psi\rangle),$$

where $|\Psi\rangle$ is any ground state, and P is the ground space projector. This, in particular, allows for the presence of long-range order in the ground states if the off-diagonal matrix elements of the local operator O are non-zero in the ground space.

It is also expected that gapped Hamiltonians are stable against local perturbations. That is, the ground state $|\Psi_t\rangle$ of $H_t = H + t \cdot V$ is expected to converge to $|\Psi\rangle$ as $t \to 0$, if V is local. Another related question is whether H_t remains gapped for small values of t. This is in fact the case, if the Hamiltonian satisfies the so-called local topological quantum order (LTQO) condition [25]. Therefore considering the set of all local Hamiltonians, the general picture is the following. There are continuous regions of gapped Hamiltonians that have exponentially decaying correlations. These gapped phases are then separated by gapless, critical Hamiltonians. These Hamiltonians typically have algebraically decaying correlations.

Phases with a degenerate ground space (and a gap above) were historically thought to be always described by symmetry breaking. This means the following: let us consider a family of Hamiltonians that depend on some parameters (and on the system size), $H(\lambda)$. The Hamiltonian commutes with a unitary U: $[H(\lambda), U] = 0$, where $U = \bigotimes_i U_i$. In the non-symmetry-broken phase, the Hamiltonian has a unique ground state and a gap above. In the symmetry-broken phase, the Hamiltonian has a degenerate ground space and a gap above. As the unitary and the Hamiltonian commute, the ground states can be chosen to be eigenstates of the unitary too. For example, consider the transverse field Ising model.

$$H(B) = -\sum_i Z_i \otimes Z_{i+1} + B \sum_i X_i.$$

This Hamiltonian commutes with the unitary $\bigotimes_i 2X_i$. If $B \gg 1$, then the Hamiltonian has a unique ground state: $|--\cdots-\rangle$. On the other hand, if $B \approx 0$, then the ground space is spanned by $|\Psi_\pm\rangle \propto |\uparrow\uparrow \ldots \uparrow\rangle \pm |\downarrow\downarrow \ldots \downarrow\rangle$. These states are also eigenstates of $\bigotimes_i 2X_i$. Note that there is long-range order in these states [26]:

$$\langle\Psi_+|Z_iZ_j|\Psi_+\rangle - \langle\Psi_+|Z_i|\Psi_+\rangle\langle\Psi_+|Z_j|\Psi_+\rangle = \frac{1}{4}.$$

Symmetry-broken phases possess local order parameters. In the above picture, one can take any local operator $\sum_i M_i$ such that e.g. $\sum_g U_g M U_g^\dagger = 0$. In this case, in the non-symmetry broken-phase, the ground state expectation value is 0: $\langle\Psi|M|\Psi\rangle = \sum_g \langle\Psi|U_g M U_g^\dagger|\Psi\rangle = 0$. In the symmetry-broken phase, on the other hand, the operator M has non-trivial matrix elements in the ground space. Therefore M distinguishes between the different ground states. In the case of the transverse-field Ising model, the local order parameter can be chosen to be the magnetization, $\sum_i Z_i$. This order parameter distinguishes between the states $|\Psi_\uparrow\rangle$ and $|\Psi_\downarrow\rangle$.

The discovery of topologically ordered systems (such as systems displaying fractional quantum Hall effect) highlighted that the above picture does not describe all phases. One of the most striking features of topological order is indeed the absence of a local order parameter: there is no local operator that distinguishes between the different ground states of the Hamiltonian. Due to this, long range order is not present in the system. Another distinctive feature of these models is that the excitations have anyonic nature. That is, the excitations of the model are point-like and moving one excitation around another might result in a phase factor different from ± 1. A consequence of this is that the ground state degeneracy depends on the topology of the surface the model is defined on.

1.2 Area law

Algorithms based on TNs are variational algorithms. But why can any variational family depending only on a few parameters represent the relevant physics if the Hilbert-space describing the joint state of N particles is exponentially large? A first answer lies in the fact that one does not need to approximate all states in the Hilbert space, but only those that are ground states of local Hamiltonians. As local Hamiltonians can be parametrized with only a few parameters (the number of parameters grows linearly with the system size), the ground states are also occupying only a small 'corner' of the Hilbert space [11]. But how to identify this relevant corner of the Hilbert space? As the obstacle behind classical understanding of strongly correlated systems is the presence of entanglement, it is natural to investigate if entanglement shows some pattern in these states. As it turns out, entanglement has a very special pattern in these states that is known as area law [27, 28]. The name area law comes from black hole physics: it was calculated that the entropy of the black hole is proportional to the area of its surface. In the context of many-body physics, the statement is the following. Consider a sub-region A of a system. Take the reduced density of the ground state, Ψ, on this region A:

$$\rho_A = \mathrm{Tr}_{A^c}\{|\psi\rangle\langle\psi|\}, \tag{1.3}$$

where A^c is the complementary region. The entanglement entropy of the state ψ with respect to this bipartition is simply the von Neumann entropy of the reduced state:

$$S_A = -\mathrm{Tr}\{\rho_A \log \rho_A\}. \tag{1.4}$$

For a gapped, local Hamiltonian with a unique ground state, the entanglement entropy S_A of the ground state is then proportional to the boundary of the region A:

$$S_A \propto |\partial A|. \tag{1.5}$$

This observation has been proven in the case of one-dimensional systems. In higher dimensions and still at zero temperature, it is conjectured (and proven under certain assumptions [29, 30]), that the area law still holds.

If the system is gapped but has multiple ground states as in the case of a topological Hamiltonian on a non-simply connected surface, the entanglement entropy has a finite correction:

$$S_A \propto |\partial A| - \log n, \tag{1.6}$$

where n is the ground state degeneracy.

In fact, even for critical systems, the area law is only violated logarithmically [31, 32]. That is, in the case of a one-dimensional critical system, the entanglement entropy S_A scales like

$$S_A \propto \log |A|. \tag{1.7}$$

This property is in sharp contrast with the fact that a random state (w.r.t. the Haar measure) has an entanglement entropy that is proportional to the volume of the region A. It suggests that entanglement is concentrated around the boundary of A. A good variational ansatz should have a similar entanglement pattern.

Chapter 2

Tensor Networks

Tensor Network states (TNs) are many-body states that admit a local description in terms of low-rank tensors. Due to the small number of parameters needed to describe them, they can be stored on a computer and used in calculations unlike the full wave function of a general state. They underlie many numerical algorithms in which they are used as variational ansatz for calculating the ground states of many-body Hamiltonians. The family of these states includes, among others, the one-dimensional ansatz of Matrix Product States (MPS) [17, 18], the higher dimensional Projected Entangled Pair States (PEPS) [19, 20], and the Multi-scale Renormalization Ansatz (MERA) [21] reflecting the scale-invariance of critical systems. One of their main feature is that the entanglement present in these states is limited through the sizes of the describing tensors leading to an area law for the entanglement entropy. This entanglement pattern is similar to that of the ground states of local Hamiltonians suggesting that they are indeed the right variational ansatzes to solve the local Hamiltonian problem.

In fact, the theory of TNs is deeply rooted in numerical algorithms designed into solve many-body Hamiltonians. One of the first numerical algorithms giving insight to strongly correlated systems is Wilson's Numerical Renormalization Group (NRG) method [33]. This method was successful in simulating certain one-dimensional problems such as the Single-Impurity Anderson Model (SIAM) [34] and the Kondo Hamiltonian [35, 36]. A necessary criterion, however, was that the Hamiltonian has a clear separation of energy scales. The Density Matrix Renormalization Group (DMRG) method [37] was able to overcome this limitation and it is thus suitable to describe any one-dimensional problem. The optimal wave functions arising from these algorithms are of the form of MPS [17], i.e. one-dimensional TNs. In fact, the DMRG algorithm can be reformulated as a variational method over MPS. As these algorithms are based on the bounded entanglement between any bipartition of the system, the area law suggests that generalization to higher dimensions is non-trivial: in two-dimensional square lattice consisting of N particles, for example, the boundary of a region can be of order $\sqrt{N}$. This extensive scaling of the entanglement causes that variational methods using PEPS are very difficult to realize. The crucial point where this manifests is that calculating expectation values of local observables is hard. Despite this fact, algorithms based on PEPS using approximate contraction routines give

now, in certain scenarios, the best known numerical results.

Another series of developments that led to the theory of TNs is coming from mathematical physics. The investigation of spin models was highly motivated by the connection of the antiferromagnetic (AF) Heisenberg model to high-T_c superconductivity. The difficulty of solving the AF Heisenberg model inspired the creation of paradigmatic wave functions for which correlations can be easily calculated. Such a paradigmatic wave function is for example given by the solution of the AKLT model [38] in one dimension. These models can shed light onto the non-trivial physics of strongly correlated systems by the creation and investigation of exactly solvable Hamiltonians for which they are the ground states. In one dimension, Finitely Correlated States (FCS) [39] generalized existing paradigmatic wave functions and allowed the investigation of these models directly in the thermodynamic limit. As MPS are finite system-size variants of FCS, many of the techniques developed for the investigation of FCS can be transferred to the analysis of MPS. In two dimensions, understanding the thermodynamic limit is more challenging. The language of TNs, in particular PEPS, however, still provides a unified language for describing exactly solvable gapped models. This includes, for instance, the Cluster State [40, 41] underlying measurement-based computation, the rotationally invariant spin-liquid AKLT [42, 38] and RVB [43] states, and other chiral [44, 45] and non-chiral states [46, 47, 48, 49] embodying topological order. In particular, PEPS encompass all known non-chiral topological orders [50]. All these states allow for the construction of local parent Hamiltonians and, by making use of their local description, the ground space structure and the behavior of the low-energy excitations can be fully analyzed.

TNS therefore seem to capture relevant physics. The understanding of these models therefore leads to new insights into how strongly correlated systems behave. In many scenarios, it turns out that TN models can be grouped into finitely many disjoint sets therefore providing a classification for these models. Such classification are, for example, the classification of gapped phases in one dimension both in the presence and absence of symmetries [23, 22], of SPT phases in two dimension [51], of Matrix Product Unitaries [52] or of RG fixed points of pure and mixed states in one dimension [52]. All these classifications rely heavily on the ability of deciding when two set of tensors generate the same TNS. Due to the importance, these kind of theorems are often referred to as Fundamental Theorems.

The goal of the rest of the chapter is to put the included publications into context. First, we introduce the widely used graphical notation of TNS. We then define some particularly important TNS, amongst them MPS and PEPS. We show then that every state can be represented as MPS (and in general, any TNS), but this representation might not be efficient. We discuss then what are the different approaches to represent states approximately as TNS providing the background needed for the publication. We then turn to the theory of translationally invariant MPS and PEPS. As the last two publications concern fundamental theorems of TNS, the goal of this part is on one hand to show how such theorems can be used in classification of models, on the other hand, to review what is already known. To demonstrate the use of fundamental theorems, we show how classification of SPT phases in one dimension works.

2.1 Graphical notation of tensor networks

Tensor Network states are quantum many-body states with special entanglement patterns. A common feature is that they describe the global wave function with the help of local components – that is, the state is described by contraction of tensors. In this Section we introduce the graphical notation standard in this field and used throughout this thesis.

Wave functions can be thought of as tensors as they are vectors in a tensor product Hilbert space. Tensors are represented by dots or boxes with lines attached to it. The lines correspond to the different indices of the tensor; joining the lines corresponds to contraction of indices. For example, a scalar is represented by a single dot with no lines joining to it, a vector is represented by a dot with a single line attached to it, a matrix by a dot with two lines attached to it:

$$s = \underset{s}{\bullet} \ , \quad |v\rangle = \overset{}{\bullet}\!\!-\!\!\underset{v}{} \ , \quad A = \overset{}{-\!\!\bullet\!\!-}\!\!\underset{A}{} \ ;$$

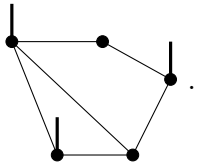
the scalar product of two vectors, the action of a matrix on a vector and a matrix element can be written as

$$\langle w|v\rangle = \underset{w}{\bullet}\!\!-\!\!\underset{v}{\bullet} \ , \quad A|v\rangle = \overset{}{-\!\!\bullet}\!\!-\!\!\underset{A}{\bullet}\!\!-\!\!\underset{v}{} \ , \quad \langle w|A|v\rangle = \underset{w}{\bullet}\!\!-\!\!\underset{A}{\bullet}\!\!-\!\!\underset{v}{\bullet} \ .$$

The wave function of a quantum many-body state then can be represented as a dot with as many lines joining to it as the number of particles:

$$|\Psi\rangle =$$  .

A state is called a tensor network state if it can be written as the contraction of smaller tensors. More precisely, given a graph, we assign to every vertex of degree d a tensor of rank d or $d+1$, where the extra index corresponds to one of the physical Hilbert spaces. The state is then obtained by contracting the indices that are connected with an edge:

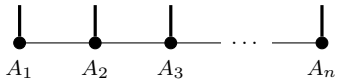
$$|\Psi\rangle =$$  .

This example is a three-partite state represented with the help of five tensors out of which three have physical indices and two do not. In the following Sections we give further examples of this construction by introducing Matrix Product States, Projected Entangled-Pair States and MERA.

2.1.1 Matrix product states

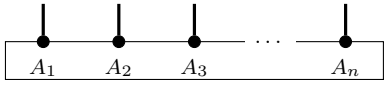
Matrix product states are the states underlying the DMRG algorithm; in fact, DMRG can be re-expressed as a variational algorithm over MPS. They can be viewed as the finite system-size variants of finitely correlated states [53]. The name itself comes from Ref. [17].

Matrix product states are tensor network states defined on a simple line:

$|\Psi\rangle =$ 

,

or a cycle (corresponding to periodic boundary conditions):

$|\Psi\rangle =$ 

. (2.1)

As each point in the graph has at most degree two, MPS have a particularly simple analytic description:

$$|\Psi\rangle = \sum_i \mathrm{Tr}\{A_1^{i_1} A_2^{i_2} \dots A_n^{i_n}\} |i_1 \dots i_n\rangle,$$

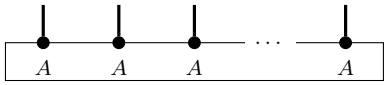
where each A_i^j is a $D_i \times D_{i+1}$ matrix. In the open boundary condition case, $D_1 \equiv D_{n+1} = 1$. An equivalent way to think of $|\Psi\rangle$ is

$$|\Psi\rangle = \sum_i |\phi^1_{i_1 i_2}\rangle \otimes |\phi^2_{i_2 i_3}\rangle \otimes \dots \otimes |\phi^n_{i_n i_1}\rangle,$$

where

$$|\phi^n_{ij}\rangle = \sum_k (A_n)^k_{ij} \; |k\rangle.$$

If all the tensors are equal in Eq. (2.1), we call the state translation invariant MPS (TI MPS). That is, a TI MPS can be written as

$|\Psi\rangle =$ 

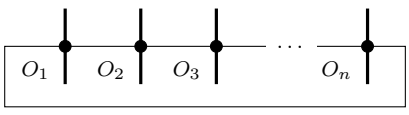
. (2.2)

An MPS tensor A defines a TI MPS for every system size. Sometimes it is necessary to emphasize the generating tensor and the system size, in this case we write $|\Psi_n(A)\rangle$ instead of just $|\Psi\rangle$.

Matrix Product Operators are operators on a tensor product Hilbert space that have MPS form. More precisely, an operator O is a matrix product operator if it can be written in the form

$$O = \sum_{i,j} \mathrm{Tr}\{O_1^{i_1,j_1} O_2^{i_2,j_2} \dots O_n^{i_n,j_n}\} |i_1 i_2 \dots i_n\rangle\langle j_1 j_2 \dots j_n|.$$

These operators can be graphically represented as

$O =$ 

.

Similar to MPS, one can define open boundary conditions and translational invariant MPOs. In fact, MPOs are just MPS with two physical indices.

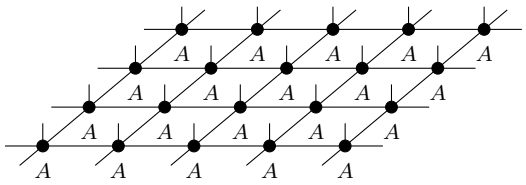
2.1.2 Projected Entangled Pair States

Projected entangled-pair states are tensor networks where each tensor has physical dimension. They can be defined using any graph. The most prominent examples are defined on a two-dimensional regular lattice, for example translation invariant PEPS defined on a square lattice. In this case, the state is defined with the help of a single rank-5 tensor:

$A =$ 

.

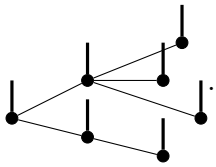
The bulk of the state then is defined by the contraction

$|\Psi\rangle =$ 

;

the boundary can either be periodic; that is, the state is defined on a torus, or defined by rank-four tensors on the sides and rank-three on the corners.

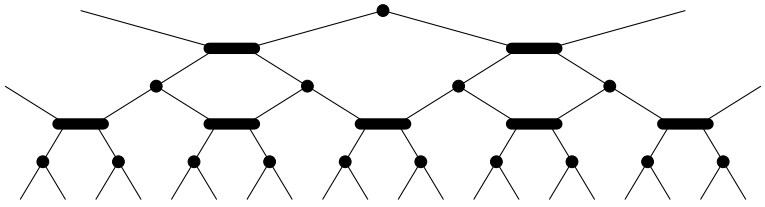
Other examples include PEPS defined on graphs that do not contain cycles: on trees. That is, the state is described as, for example,

$|\Psi\rangle =$ 
.

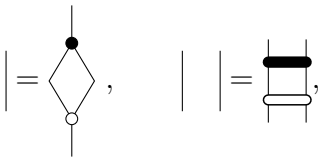
In this case, the lack of cycles means that the calculation of expectation values is simple. The underlying geometry, however, restricts their representation power. One of their possible uses is in quantum chemistry as a post Hartree-Fock method. Here, the different tensors represent different modes. The geometry of the network is then determined by the strongest correlations between the different modes in a simple approximation; these correlations are found to be robust, and thus the geometry calculated from the simpler approximation works well.

2.1.3 Multi-scale renormalization ansatz

The multi-scale renormalization ansatz is a TN ansatz that reflects the scale-invariance of critical systems. One-dimensional MERA is defined with the help of rank-three and rank-four tensors in the bulk as



The rank-three tensors are required to be isometries while the rank-four tensors unitaries:



where the white filling denotes taking the adjoint (complex conjugation and reverse reading direction).

2.2 Representing states as TNS

Tensor Networks are widely used as variational ansatzes in numerical algorithms. As such, it is crucial to understand how well can TNS describe states. We show that every state can be represented as non-TI MPS and PEPS. The bond dimension (and thus the number of parameters) required for the description, however, generally scales exponentially with the system size.

Despite this general exponential scaling, MPS and PEPS are good ansatzes for describing ground and thermal states of local Hamiltonians. This is closely related to the area law: the entanglement present in the aforementioned states is localized at the boundary for any bipartition.

2.2.1 Exact representation of states

One of the evidences that MPS is a good variational ansatz is that every state can be represented as open boundary condition (OBC) non-TI MPS [54]. We shortly review the proof as it also explains which states can be *efficiently* approximated as MPS. Let $|\Psi\rangle$ be a state on n particles arranged in a line. Let a minimal-rank decomposition corresponding to the cut between particle i and $i+1$ be

$$|\Psi\rangle = \sum_j |\phi_j^i\rangle \otimes |\xi_j^i\rangle.$$

Notice that for every $i < n-1$, one can write

$$|\xi_j^i\rangle = \sum_k |\psi_{jk}^{i+1}\rangle \otimes |\xi_k^{i+1}\rangle \tag{2.3}$$

for some vectors $|\psi_{jk}^{i+1}\rangle$, as on the last $n-i-1$ particles, $|\Psi\rangle$ is completely supported on the vectors $|\xi_j^{i+1}\rangle$. Therefore, starting from the left, the state $|\Psi\rangle$ can be written as

$$|\Psi\rangle = \sum_k |\phi_k^1\rangle \otimes |\xi_k^1\rangle = \sum_k |\phi_{k_1}^1\rangle \otimes |\psi_{k_1 k_2}^2\rangle \otimes |\xi_{k_2}^2\rangle.$$

Continuing the process by repeatedly using Eq. (2.3) leads to the MPS form

$$|\Psi\rangle = \sum_k |\phi^1_{k_1}\rangle \otimes |\psi^2_{k_1 k_2}\rangle \otimes \cdots \otimes |\psi^{n-1}_{k_{n-2} k_{n-1}}\rangle \otimes |\xi^{n-1}_{k_{n-1}}\rangle.$$

This shows that for exact representation of the state, the minimal bond dimension required at any given cut is exactly the Schmidt rank of the state for the corresponding bipartition. As for general n-partite states the Schmidt rank at the cut in the middle of the chain grows exponentially with n, this representation is not efficient.

Note that the above argument can readily be generalized for PEPS defined on a tree. That is, any state can be written as a PEPS defined on a tree. Let us consider now PEPS defined on an arbitrary graph. Note that removing an edge from the graph means setting the corresponding bond dimension to one and thus removing an edge from the underlying graph decreases the representative power of the ansatz. As every graph contains a tree, every state can be represented as PEPS independent of the underlying graph. The bond dimension needed for this representation, however, might scale exponentially with the number of particles, which makes this statement unpractical. The important question is to understand what is the representative power of tensor networks with low bond dimension (that is, at most polynomially scaling with the system size).

2.2.2 Approximating states

Tensor Networks are used in variational algorithms to find ground states of many-body Hamiltonians. It is therefore important to understand what are the limitations of the ansatz: which states can be approximated as TNS with a small number of parameters.

To formalize the question, notice that the important thing is how the bond dimension scales with the number of particles. That is, consider a family of states, $|\Psi_N\rangle$, where the index N stands for the number of particles. Fix an error ϵ, and look for the lowest bond dimensional TNS, $|\tilde{\Psi}_N\rangle$, such that the distance between $|\Psi_N\rangle$ and $|\tilde{\Psi}_N\rangle$ is smaller than ϵ. The question is then how the bond dimension D_N of $|\tilde{\Psi}_N\rangle$ scales with N.

First, it is important to clarify what is a good approximation; that is, what distance measure we use to quantify closeness of states. Even though in a finite dimensional vector space every norm is equivalent, the different norms might scale differently with the number of particles and thus using different norms leads to qualitatively different results.

A very natural choice is to require that the approximation is ϵ-precise for every *local* observable. Let us require for example that it is ϵ-precise for every observable on neighboring particles. That is, if the reduced density of $|\Psi_N\rangle$ and $|\tilde{\Psi}_N\rangle$ on particles i and $i+1$ is $\rho^N_{i,i+1}$ and $\tilde{\rho}^N_{i,i+1}$ correspondingly, then this approximation naturally leads to the condition

$$\|\rho^N_{i,i+1} - \tilde{\rho}^N_{i,i+1}\|_1 \leq \epsilon.$$

Note that this approach only makes sure that the expectation values of local observables are well approximated, thus expectation values of global operators such as the Hamiltonian, might have an extensive error. That is, even if the Hamiltonian is a sum of local terms,

the energy difference of $|\Psi_N\rangle$ and $|\tilde{\Psi}_N\rangle$ might scale with N and thus $|\tilde{\Psi}_N\rangle$ might have very small overlap with the actual ground state $|\Psi_N\rangle$. In order to obtain a good overlap, one has to take an approximation error ϵ that scales as the inverse of the system size. This approach is taken, for example, in [55].

Another possibility for approximating a many-body state is to require that expectation values of *every* (even multi-particle) observable is precise up to error ϵ. This leads to an approximation in the one-norm:

$$\sup_{\|O\|=1} \left| \langle \Psi_N | O | \Psi_N \rangle - \langle \tilde{\Psi}_N | O | \tilde{\Psi}_N \rangle \right| = \left\| |\Psi_N\rangle\langle\Psi_N| - |\tilde{\Psi}_N\rangle\langle\tilde{\Psi}_N| \right\|_1 \leq \epsilon. \tag{2.4}$$

This approximation scheme is present in many papers, including Refs. [56, 57, 1, 58].

Approximation with TNS has been analyzed in several papers [59, 55, 58]. The best bounds are found for MPS, where fast decaying Schmidt coefficients mean good approximation. This, in fact, can be proven with similar tools as the area law, even though an area law for the von Neumann entropy only does not mean approximability with MPS [60]. For PEPS, all known bounds are worse [56, 57]. We analyze this problem in Section 3.1.

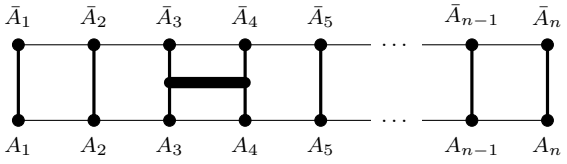
2.3 Expectation values

As TNS are used as variational ansatz, it is important to be able to calculate the energy of a given TNS. The Hamiltonians in consideration are local Hamiltonians, thus one needs to calculate the expectation value of local observables. This expectation value can be expressed as the contraction of a tensor network without physical indices. This problem is easy in 1D, while very complicated in 2D; that is the reason behind the success of DMRG and why calculations with PEPS are so difficult.

2.3.1 MPS: transfer matrix

We demonstrate with the help of MPS how the calculation of expectation values reduces to the contraction of a tensor network without physical symmetries. In the translation invariant case, this contraction can be expressed as the trace of the powers of a completely positive (CP) map called the transfer operator.

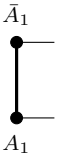
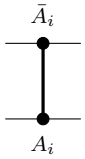
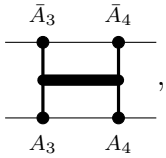
Let O be a two-local operator. Then the expectation value $\langle \Psi | O | \Psi \rangle$ can be graphically represented as:

$\langle \Psi | O | \Psi \rangle =$ 

.

This expression can be evaluated efficiently if it is evaluated from left to right. In this way,

in each step one has to store a matrix of $D^2 \times D^2$ dimension: define

$E_1 =$  , $E_n =$  , $E_i =$  , $X =$  ,

then the expectation value can be expressed as

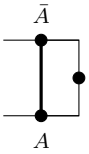
$$\langle \Psi | O | \Psi \rangle = E_1 \cdot E_2 \cdot X \cdots E_n.$$

That is, the expectation value is simply the product of n matrices and thus can be calculated even for a very long chain (if the bond dimensions are bounded).

In the translationally invariant case, the matrices E_i all coincide and the expectation value takes the form

$$\langle \Psi | O | \Psi \rangle = \mathrm{Tr}\{X \cdot E^n\}.$$

One can think of the matrix E as a linear operator with action

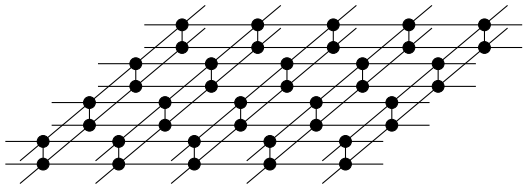
$\rho =$  $\mapsto E(\rho) = \sum_i A_i^\dagger \rho A_i =$  . (2.5)

E is called transfer matrix and it is a CP map. Spectral properties such as primitivity, irreducibility and reducibility of this map tell a lot about the MPS itself such as how to decompose it into a sum of simpler MPS.

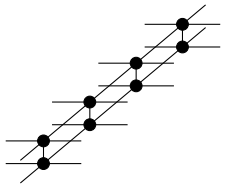
2.3.2 PEPS

Higher-dimensional tensor networks are less successful then their one-dimensional counterparts. This is caused mainly by the fact that calculating expectation values is difficult. In recent years, however, there has been a significant development that made algorithms based on PEPS be able to outperform other conventional methods such as quantum Monte Carlo sampling. In this section, we show why the contraction of PEPS is difficult.

Similar to MPS, expectation values of local observables can be expressed as a contraction of a tensor network without physical indices. The difference, however, is that this tensor network is two-dimensional. For example, the norm of a PEPS defined on a two-dimensional square lattice can be represented as

$\langle \Psi | \Psi \rangle =$  .

The problem with contracting an $n \times m$ PEPS is the following. If one contracts from left to right, at each step one has to store a vector that is defined on m particles. That is, the transfer matrix is defined on multiple particles:

$T =$  .

At the beginning of the contraction, one can store this vector due to its MPS form. After every new line contracted, the result is still an MPS, its bond dimension, however, might grow exponentially with the number of rows contracted. The exponential scaling of the bond dimension makes this process unfeasible. It has been shown that this intuition is accurate: contracting PEPS is a very hard ($\#P$-hard) [61].

The root of the problem is the presence of loops in the graph on which the PEPS is based. Indeed, in the case of a PEPS defined on a tree the contraction is easy by recursion: the leaves (degree-one vertices) can always be removed from the graph. This makes tree tensor networks highly suitable for numerical simulations [62].

In practice there are several methods to circumvent the problem. This of course requires approximate contraction schemes. Such scheme is the corner transfer matrix method used to contract TI PEPS on square lattices. Here, the contraction is reduced to finding the solution of a fixed-point equation.

2.4 Decomposition into simple objects

One of the most important features of TI MPS is that it can be decomposed into the sum of smaller TI MPS. This, together with the understanding of the indecomposable objects – called *normal* MPS – leads to the understanding of general MPS: which parameters in the describing tensor are irrelevant and what are the remaining degrees of freedom in describing a given state. These theorems are often referred to as fundamental theorems and are discussed in Section 2.7.

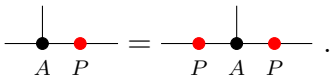
While the theory of MPS is successful mainly due to the possibility to decompose MPS into a sum of simple objects, a similar theory is still missing for PEPS. The definition of *normality* can, however, be generalized to this situation as well. It is partially due to the lack of this decomposition that fundamental theorems are only known to very restricted classes of PEPS.

2.4.1 Structure of TI MPS

The decomposition of TI MPS into simple objects is based on finding invariant and periodic (invariant after blocking) subspaces of the MPS tensors. We prove that if an invariant (or periodic) subspace can be found, then the MPS can be written as the sum of two (or more)

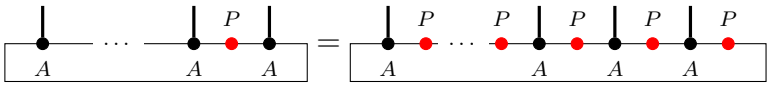
smaller bond dimensional MPS. Note that this does not mean that the MPS tensor itself is the direct sum of the two smaller MPS tensors: it might only be upper or lower block triangular. Once all invariant and periodic subspaces are found, the remaining tensor is a normal tensor and thus the building blocks of TI MPS are normal MPS. We also prove that the decomposition obtained above is unique (on the level of states).

The first important step in the decomposition of TI MPS is to find invariant subspaces. That is, given an MPS tensor A with the help of the matrices $A^i \in \mathcal{M}_D$, to find a vector space $V \subseteq \mathbb{C}^D$ such that $V = \mathrm{Span}_i\{A^i V\}$. If P is a projector onto V, this means that the MPS tensor A satisfies $A^i P = P A^i P \ \forall i$, or graphically



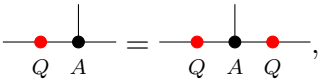
(2.6)

Inserting P on one of the bonds of the MPS is the same as inserting P on every bond:

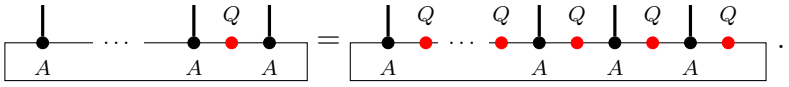


(2.7)

as it can be seen using Eq. (2.6) repeatedly. It can also be seen that Eq. (2.6) is equivalent to

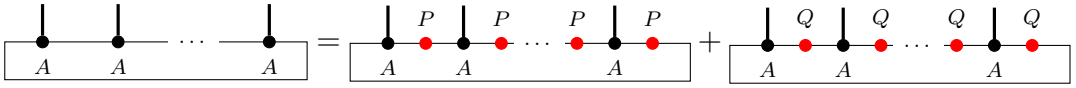


for $Q = 1 - P$, and thus inserting Q on one of the bonds is the same as inserting it on all of the bonds:



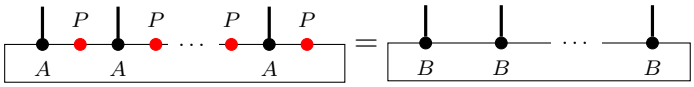
(2.8)

This means that if such a projector can be found, the MPS decomposes into the sum of two MPS:



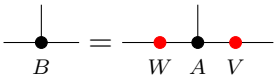
(2.9)

These two MPS, moreover, can be written as smaller bond dimensional MPS: let the rank of P be $r < D$. If $P = VW$ is a decomposition of P with $W : \mathbb{C}^D \to \mathbb{C}^r$ and $V : \mathbb{C}^r \to \mathbb{C}^D$, then



(2.10)

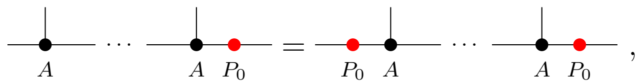
where



(2.11)

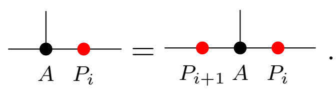
This process then leads to the decomposition of the TI MPS into smaller bond dimensional TI MPS, and thus can be continued until there can be no more invariant subspaces found.

Even if there are no more invariant subspaces present in the MPS tensor, there might still be invariant subspaces *after blocking*. We call such a subspace periodic subspace. Let V_0 be any subspace, and let us define V_i by the recursion $V_{i+1} = \mathrm{Span}_j\{A^j V_i\}$. Then V_0 is a periodic subspace if there is n for which $V_n = V_0$. If P_0 is a projector onto V_0, then



(2.12)

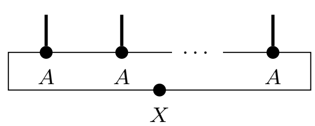
and thus the MPS can be decomposed as a sum of smaller bond dimensional MPS *after blocking* using the method above. Note that if V_0 is a minimal periodic subspace, then $V_0 \cap V_k = 0$ for all $k = 1...(n-1)$, as that subspace is also invariant after blocking n tensors. Therefore if P_i projects onto V_i and $P_i P_j = 0$, then $\sum_i P_i = 1$ (due to the lack of invariant subspaces) and



(2.13)

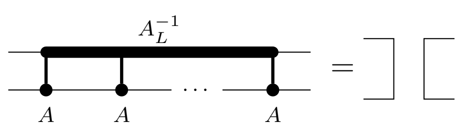
This shows that the MPS takes value zero for every system size that is not a multiple of n. If the system size is a multiple of n, then the MPS is the sum of n indecomposable MPS.

Suppose now that there are no invariant or periodic subspaces in A. Then in Ref. [63] it has been proven that A is *normal*, that is, there is an L such that L consecutive tensors satisfy



$$= 0 \quad \Rightarrow \quad X = 0. \tag{2.14}$$

L is called the injectivity length and if the tensor A is normal with $L = 1$, then it is called *injective*. Note that normal tensors, after blocking, have one-sided inverses:

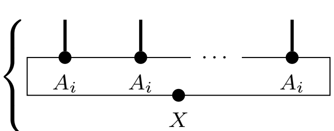


(2.15)

We have therefore proven that any TI MPS, after blocking, is a sum of normal TI MPS. This decomposition is unique due to the orthogonality of normal MPS in the thermodynamic limit: if A and B are normal tensors, then either $|\Psi_n(A)\rangle = \lambda^n |\Psi_n(B)\rangle$ or

$$\frac{|\langle \Psi_n(A)|\Psi_n(B)\rangle|^2}{\|\Psi_n(A)\|^2 \cdot \|\Psi_n(B)\|^2} \to 0 \tag{2.16}$$

as $n \to \infty$ [52]. This means that given a set of normal tensors $\{A_i\}$, there exists N such that for all $n > N$ the states $|\Psi_n(A_i)\rangle$ are linearly independent, and thus the decomposition above is unique. Actually, with the same proof it can be shown that given different normal MPS described by tensors A_i, the vector spaces

$V_i = \Bigg\{$  $\Bigg| \; X \in \mathcal{M}_D \Bigg\}$

are linearly independent for large enough n.

Note that the existence of invariant and periodic subspaces is related to the spectral properties of the transfer matrix.

Definition 1. A CP map T is *primitive* if there is an n such that $T^n(\rho) > 0$ (that is, it is strictly positive) for any $\rho \geq 0$ (that is, positive semidefinite) [64]. It is *reducible* if there is a projector $P \geq 0$, $P \neq 0$, $P \neq \mathrm{Id}$ such that $T(P) \leq \lambda P$. It is *irreducible* if it is not reducible and it is *periodic* if it is irreducible but not primitive.

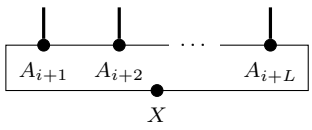
To connect these definitions with spectral properties, first note that the Perron-Frobenius theorem states that for any CP map T with spectral radius 1, 1 is an eigenvalue and there is a corresponding eigenvector that is positive semi-definite. That is, there is $\rho \geq 0$ such that $T(\rho) = \rho$. The following theorem shows how the above properties of T are reflected in its spectrum:

Theorem 1. *Suppose the CP map T has spectral radius 1. Then T is primitive if and only if 1 is the only eigenvalue with absolute value 1, it has multiplicity 1 and the corresponding eigenvector is positive definite. If T is periodic, the eigenvalues with absolute value 1 are p-th root of unity for some p.*

Given an MPS tensor A, the corresponding transfer matrix T is reducible if and only if there are invariant subspaces. T is periodic if and only if there are no invariant subspaces but there are periodic subspaces. Finally, A is normal if and only if T is primitive [63].

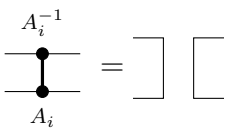
2.4.2 Non-TI MPS

For non-TI MPS no similar decomposition is known. More precisely, one has to be careful when formulating a similar theorem: the expansion of an MPS in any product basis is a sum of product states and thus a sum of normal MPS. This expansion is, however, not interesting due to the large number of terms. Despite that, several notions can be transported from the TI case; for example, periodic/invariant subspaces can be found (these two notions are the same in the non-TI case). Similarly, the notion of injectivity and normality can be generalized to the non-TI case. A non-TI MPS is called normal, if after blocking any L consecutive tensors, the following holds:



$$= 0 \quad \Rightarrow \quad X = 0. \tag{2.17}$$

If $L = 1$, the MPS is called injective. That is, an MPS is injective if all tensors have an inverse:

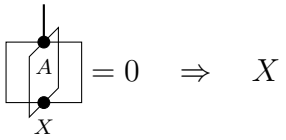


(2.18)

2.4.3 PEPS

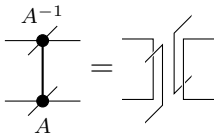
Similar to the non-TI MPS case, it is not known whether PEPS can be decomposed into the sum of simple objects (apart from the expansion in a basis). However, the notions of injectivity and normality can be generalized to PEPS as well.

A PEPS tensor A is injective if as a map from the virtual to the physical state it is injective:



$$= 0 \quad \Rightarrow \quad X = 0. \tag{2.19}$$

This is equivalent to the tensor A admitting a one-sided inverse A^{-1}:

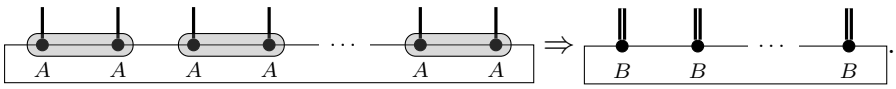


(2.20)

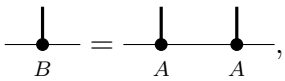
Similar to the MPS case, a PEPS tensor is called normal, if it becomes injective after blocking in a finite, simply connected region such as in a rectangle. These notions can be generalized to the non-translationally invariant setting.

2.5 Renormalization

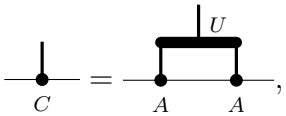
An important concept is that of *renormalization*. The renormalization process consists of two steps: blocking and applying an isometry that reduces the physical dimension. The blocking step is easily represented by the blocking of tensors:



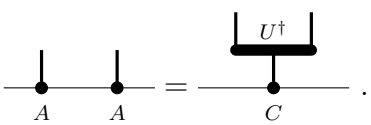
Notice that the tensor B, obtained by blocking two (resp. n) A tensors:



is defined on the physical Hilbert space $\mathcal{H} \otimes \mathcal{H}$, but it only spans a bounded-dimensional subspace of it no matter how many tensors we block. There is thus an isometry that does not 'change the state' but maps it back to a bounded-dimensional Hilbert space:

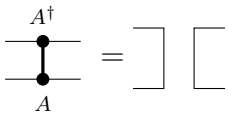


(2.21)



(2.22)

This is the second step of the renormalization process. If the bond dimension of the tensor A is D, then the physical dimension of C is at most D^2. The bond dimension of C is the same as that of A, thus repeating the renormalization step always results in states with physical dimension at most D^2. That is, for MPS, one can define a renormalization process. This process does not affect the decomposition into normal MPS. In fact, the renormalization fixed points are exactly those MPS that are sums of pairwise locally orthogonal injective *isometric* MPS [52]; injective isometric MPS are described in terms of isometries: the defining tensor A satisfies



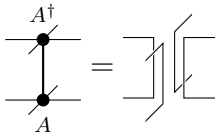
(2.23)

Note that injective isometric MPS have zero correlation length as expected from (gapped) renormalization fixed points.

2.5.1 PEPS

Renormalization for PEPS is more difficult; in fact, there is no known procedure for that. One way around this is to use the bulk-boundary correspondence and renormalize MPOs describing the boundary of the system; this approach is taken in Ref. [52].

Note that any gapped renormalization fixed point has zero correlation length. In case of unique ground states, it means that the state can be written as some local isometries acting on product states; the product structure of these two layers, however, might be non-overlapping. Such states are, for example, injective isometric PEPS; these are PEPS where the PEPS tensors satisfy



(2.24)

Other examples include isometric semi-injective PEPS as defined in Section 3.3. These states also have the two-layer structure described above.

2.6 Virtual symmetries and topological order

The decomposition of TI MPS leads to the identification of a special class of MPS tensors. These MPS tensors can be characterized as the centralizer of the group algebra of a finite group G. The class of MPS obtained this way is then called G-injective MPS. The concept of G-injectivity can then be generalized to PEPS. We show that the presence of the virtual symmetries leads to a set of locally indistinguishable states characteristic for topological order.

The above concepts can be further generalized leading to MPO-injective PEPS. We do not include the the description of MPO-injective PEPS in this thesis. For MPO-injective

PEPS tensors, the virtual symmetries are described with the help of some special MPOs instead of the tensor product of group elements. This class of tensors is capable to describe every known topological lattice models (that is, it can describe all string-net models).

2.6.1 G-injective MPS

Let A be an MPS tensor. Using the decomposition from Section 2.4, we can give another MPS tensor B that – after blocking enough particles – generates the same state as A, yet has a much simpler form. To do that, notice that after blocking, A is just the sum of injective MPS; B is then just the direct sum of these components:

$$B^i = \bigoplus_j \mathrm{Diag}\left(\lambda_1^{(j)}, \ldots, \lambda_{m_j}^{(j)}\right) \otimes A_j^i, \tag{2.25}$$

where the j^{th} normal MPS appears m_j times in the decomposition, with weights λ_j. Using the orthogonality of normal MPS, we see that – after blocking – the matrices B^i span all such block diagonal matrices:

$$\mathrm{Span}_i\{B^i\} = \bigoplus_j \mathrm{Diag}\left(\lambda_1^{(j)}, \ldots, \lambda_{m_j}^{(j)}\right) \otimes \mathcal{M}_{d_j}.$$

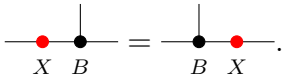
A subset of these tensors, where all $\lambda_i^{(j)}$ are equal for a given block j, is particularly appealing. These tensors are in the form

$$B^i = \bigoplus_j \mathrm{Id}_{m_j} \otimes A_j^i,$$

and the matrices B_i span every matrix of this form. Notice that this block diagonal form means that virtual symmetries are present. In fact, B^i is just the centralizer of the algebra

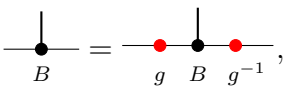
$$\mathcal{A} = \bigoplus_j \mathcal{M}_{m_j} \otimes \mathrm{Id}_{d_j}. \tag{2.26}$$

That is, for all $X \in \mathcal{A}$,

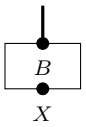


(2.27)

Notice that the algebra $\mathcal{A}$ can be thought of as a representation of the group algebra of a finite group G. With this, the symmetries of B are completely determined by the representation of the group elements:

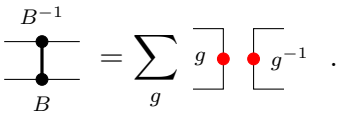


and for any matrix $X \in \mathcal{M}_D$,



$$= 0 \quad \Rightarrow \quad \sum_g g^{-1} X g = 0,$$

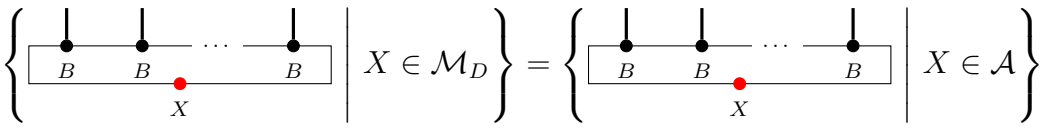
as $X \mapsto \sum_g g^{-1} X g$ is the projector onto the symmetric part of X. These two properties are called G-injectivity and the second condition is equivalent to the the existence of the pseudo-inverse B^{-1} satisfying:



(2.28)

A tensor is then called G-normal if it is symmetric and after blocking it becomes G-injective. G-injectivity and G-normality can be defined for non-TI MPS, too.

Note that the states

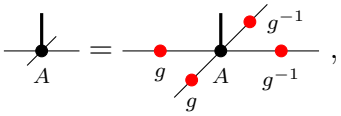


generate the subspace spanned by all different MPS present in the decomposition, defined by tensors A_j. These basis vectors are then *locally* distinguishable.

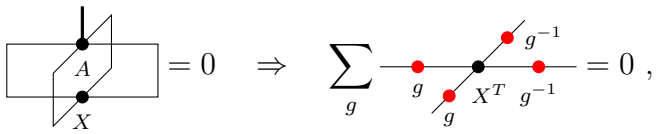
2.6.2 G-injective PEPS

G-injectivity and G-normality can be defined for PEPS as well. Contrary to the MPS case, one can create *locally indistinguishable* states using G-injective tensors and thus represent topologically ordered subspaces with it. Note that these states do not represent all known topologically ordered lattice models. To write all such states (i.e., all string-net models) as PEPS, one needs to use a generalization of G-injectivity called MPO-injectivity.

A G-injective PEPS tensor is a PEPS tensor satisfying two properties. First, it is symmetric:

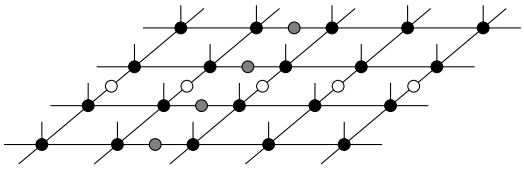


second, it is completely supported on the trivial subspace:

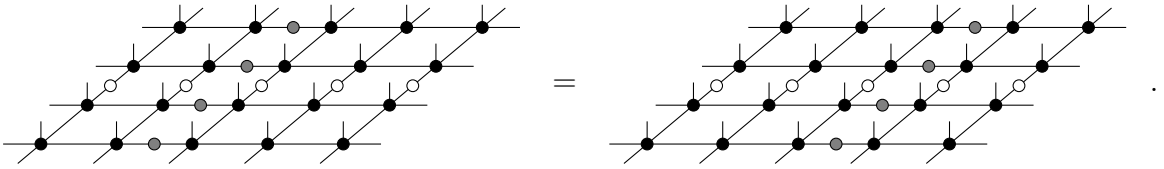


where X^T means that it is transposed both in vertical and horizontal directions. G-normality can be defined by requiring on one hand that the tensor is symmetric, on the other hand that the full support condition holds after blocking. Similar to the MPS case, both G-injectivity and G-normality can be defined for the non-TI setting, and, in fact, for any geometry.

Similar to the MPS case, one can consider the states obtained by inserting group elements before closing the boundary. More precisely, consider the states labeled by two commuting group elements g and h that are defined as

$|\Psi_{g,h}\rangle =$  ,

where the white tensors correspond to the group element g while the gray ones to the group element h. We consider the state with closed boundary – that is, on a torus – and thus the strings of two group elements form the two non-equivalent incontractible loops. The string of g (and h) can be deformed arbitrarily and can thus be moved through the lattice (in the case of $[g, h] = 0$):



Note that the states $|\Psi_{g,h}\rangle$ and $|\Psi_{g',h'}\rangle$ are the same if there is a group element k such that $g' = kgk^{-1}$ and $h' = khk^{-1}$. Therefore the dimension of this subspace can be counted as follows. Take all pairs (g, h) such that $[g, h] = 0$. Consider the equivalence relation $(g, h) \equiv (kgk^{-1}, khk^{-1})$ on this set. The number of linearly independent states is then the number of such equivalence classes (in case the representation of the group algebra is faithful). This number can be shown to be the same as the number of irreducible representations of the Drinfel'd double of the group algebra $\mathbb{C}[G]$.

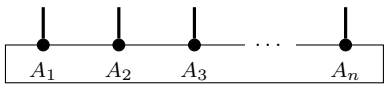
The set of states defined above can be shown to have topological properties. First, these states, unlike in the case of MPS, are indistinguishable by local operators – at least in the G-isometric case [46]. Second, the ground-state degeneracy depends on the genus of the surface the model is defined on. For this, note that as G-injectivity can be defined for any lattice geometry, one can define a similar model on the sphere, too. There are no incontractible loops on the sphere, thus the loops above can be moved to a single point, where they vanish.

2.7 Fundamental theorems

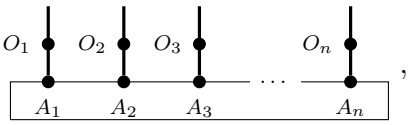
Certain operations do not change the entanglement structure of states, and thus bring TNS to TNS. Such operations include local operators, time reversal symmetry (conjugation), translation and reflection symmetries. After these operations, the state is described by some other tensors that are related to the original ones. If any of the above operations is a symmetry of the given TNS, then we arrive at two different sets of tensors describing the same state. To understand how to represent symmetric TNS it is therefore fundamental to

understand how two sets of tensors can generate the same state. In this Section we provide an overview of the relevant questions and the existing theorems.

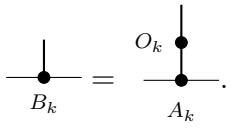
Let us first show that the symmetries listed above bring TNS to TNS. For example, if a state is represented by an MPS,

$|\Psi\rangle =$ 

then the state $\bigotimes_i O_i|\Psi\rangle$ can be written as

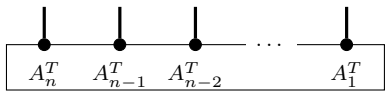
$\bigotimes_i O_i|\Psi\rangle =$ 

and thus the state after applying local operators admits an MPS description with tensors



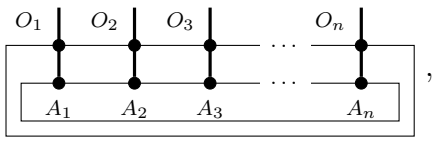
(2.29)

Similarly, the reflection of the state can be written as

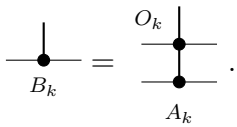
$R|\Psi\rangle =$ 

Not only do these states not change the MPS (or similarly, PEPS) form, but they also leave properties such as injectivity, normality and G-injectivity invariant. In one dimension, the decomposition into normal MPS is also invariant.

More generally, if an operator can be expressed as a TN, it also transforms TNS to TNS, but with increased bond dimension. For example, an MPO acting on an MPS,

$O|\Psi\rangle =$ 

is also an MPS that is described with the tensors



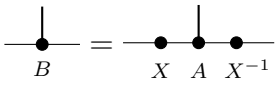
(2.30)

Unlike the above simple operations, these operations in TN form do not leave properties like injectivity, normality or G-injectivity invariant. Moreover, in one dimension, they might change the decomposition into normal MPS.

2.7.1 Fundamental theorems for TI MPS

The one-dimensional case is relatively simple due to the decomposition into normal MPS. Because of the existence of such a decomposition, one just have to prove the Fundamental Theorem for normal MPS.

Two normal MPS tensors A and B generate the same state (for system sizes $N \geq 2L+1$) if and only if they are related by a gauge (see also Section 3.5):



(2.31)

For general TI MPS, we have a similar statement if it is in block-diagonal form with normal components. In this case, one has to assume that the two MPS generate the same state for every system size. Then, if both tensors are in the form of Eq. (2.25), that is,

$$A^i = \bigoplus_j \mathrm{Diag}\left(\lambda_1^{(j)}, \ldots, \lambda_{m_j}^{(j)}\right) \otimes A_j^i, \tag{2.32}$$

$$B^i = \bigoplus_j \mathrm{Diag}\left(\mu_1^{(j)}, \ldots, \mu_{k_j}^{(j)}\right) \otimes B_j^i, \tag{2.33}$$

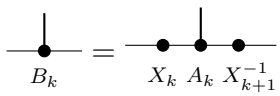
the MPS generated is the sum of the individual components:

$$|\Psi_N(A)\rangle = \sum_j \sum_{i=1}^{m_j} \left(\lambda_i^{(j)}\right)^N |\Psi_N(A_j)\rangle, \tag{2.34}$$

$$|\Psi_N(B)\rangle = \sum_j \sum_{i=1}^{k_j} \left(\mu_i^{(j)}\right)^N |\Psi_N(B_j)\rangle. \tag{2.35}$$

Therefore, by the orthogonality of MPS in the thermodynamic limit, for each j there is a k such that A_j and B_k are related by a gauge. Moreover, if the states are the same for every N, then the prefactors λ and μ coincide. Therefore there is a global gauge relating the two tensors [52]. Finally, a similar statement can be obtained if the components are allowed to be periodic, not only normal [65].

For non-TI MPS with open boundaries, a similar statement was proven in Ref. [66]. For periodic boundaries, one has to require that both of the MPS are normal, see Section 3.5. In the non-TI case, the gauge might depend on the position. That is, for every k,

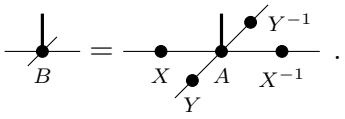


(2.36)

2.7.2 PEPS

For PEPS, proving fundamental theorems is more difficult. In fact, such theorems only exist for normal tensors. The difficulty of the general case is related to the lack of the ability to decompose PEPS into a sum of simple objects.

Two normal tensors A and B generate the same state if and only if (provided that the system size is large enough) they are related to each other as [67]:



For general tensors, however, the above equation does not hold. There are explicit counterexamples presented in Ref. [2], see Section 3.3. In this case, not local gauges but an MPO on the boundary relates the two tensors. The situation is in fact even worse: it is in general undecidable whether two PEPS tensors generate the same state [6].

It is therefore important to find classes of tensors for which the question is decidable. Apart from the normal case, another example of such a class is presented in Ref. [2], see Section 3.3. This class of tensors is a generalization of injective PEPS and can be used for a deeper understanding of SPT classification. It is also conjectured that G-injective and MPO-injective tensors generating models that display topological order are such classes. As a step towards a Fundamental Theorem for these tensors, we reprove the Fundamental Theorem for injective and normal tensors. The proof is significantly different from the already existing proof of Ref. [67]. This difference allows us to generalize to the non-translationally invariant case as well as for arbitrary geometry.

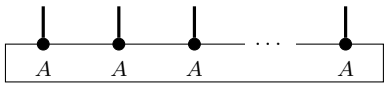
2.8 Parent Hamiltonians

Given a TNS, one can systematically construct a frustration-free Hamiltonian such that the given state is its ground state. This Hamiltonian has a ground space described in Section 2.6. This Hamiltonian can thus display topological order. Moreover, in the isometric case, the Hamiltonian is a sum of commuting terms as expected in renormalization fixed points.

2.8.1 MPS

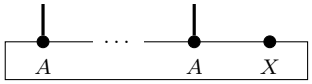
In this Section, we demonstrate the parent Hamiltonian construction with the help of MPS. We point out that in the G-injective case the ground space degeneracy is a result of symmetry breaking. Consider a translationally invariant MPS defined by a tensor A:

$$|\Psi\rangle =$$



Le us consider the n-particle subspace that is generated locally by the tensor A:

$$S = \left\{ \right.$$



$$\left. \middle| \; X \in M_{D\times D} \right\} .$$

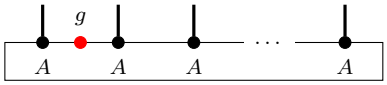
The Hamiltonian term is given as the projector onto the orthogonal subspace of S: $h = Proj(S^{\perp})$. Then the full Hamiltonian is the sum of all translations τ of this term:

$$H = \sum_n \tau^n(h). \tag{2.37}$$

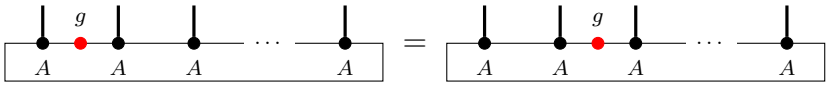
This Hamiltonian is a positive operator as it is the sum of Hermitian projectors. The state $|\Psi\rangle$ has zero energy, thus it is a ground state.

If, moreover, the tensor A is injective, then it is enough to consider the Hamiltonian for $n = 2$; this Hamiltonian contains only nearest neighbor terms. It can be shown that the Hamiltonian has a unique ground state and that it is gapped. If A is normal, then to obtain this unique ground state, one has to consider the construction for $n > 2$. If A gets injective after blocking L sites, then it is enough that the Hamiltonian terms act on $L + 1$ particles.

For G-injective MPS, it can be shown that the ground space of the Hamiltonian is spanned by the elements

$|\Psi_g\rangle =$ 

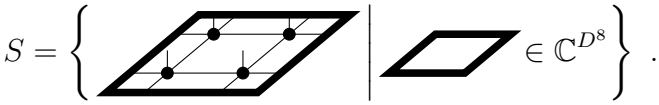
Note that as the element g moves through the network,

$|\Psi_g\rangle =$ 

it is easy to see that these elements are all ground states and, in fact, these are the only ones [66, 46]. Out of these elements, $|\Psi_g\rangle$ and $|\Psi_h\rangle$ describe the same state if and only if $h = kgk^{-1}$. Therefore, the ground-state degeneracy is the number of conjugacy classes in G. These states can be locally distinguished and thus the ground-state degeneracy of the Hamiltonian comes from symmetry breaking.

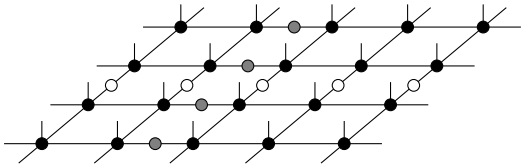
2.8.2 PEPS

In this Section, we show how the parent Hamiltonian construction for MPS generalizes to PEPS. Consider a TI PEPS defined on a square lattice. A four-body Hamiltonian term can be defined as a projector onto the subspace

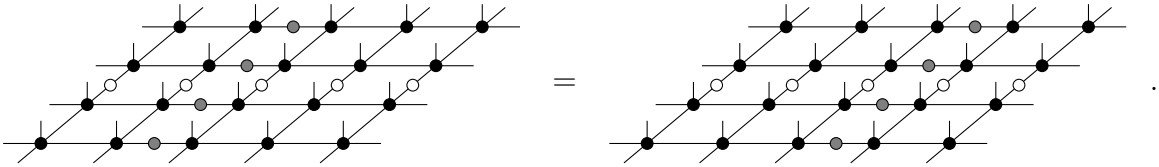
$S =$ 

Similar to the MPS case, the parent Hamiltonian of injective PEPS have a unique ground state for any finite size (and periodic boundary conditions), but it is not necessarily gapped and thus the ground-space might be degenerate in the thermodynamic limit [68].

In the G-injective case, the Hamiltonian might display topological order. In this case, the ground states might be labeled by two commuting group elements g and h and are defined as

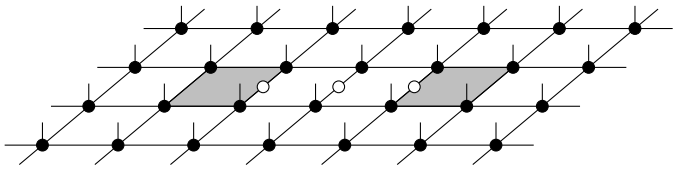
$|\Psi_{g,h}\rangle =$  ,

where the white tensors correspond to the group element g while the gray ones to the group element h. These states look locally like the state $|\Psi\rangle$ as the line of g can be deformed arbitrarily and can thus be moved through the lattice (for that , $[g, h] = 0$ is also required):



As shown in Section 2.6, some of these states coincide. The resulting ground state degeneracy then depends on the topology of the surface on which the model was defined.

The excitations of these models are anyonic excitations. For example, two magnetic fluxes located at the gray rectangles are described by

 .

2.9 Phase classification

In this Section we demonstrate how Tensor Networks can be used for phase classification. The philosophy behind this classification is the following. TNS are expected to approximate ground states of gapped Hamiltonians well. These states also possess parent Hamiltonians. It is known that any two parent Hamiltonian of a given state are in the same phase; we therefore classify the parent Hamiltonians of TNS. A particularly nice feature of this approach is that due to the fundamental theorems we know how symmetries of the state emerge from their local description and thus it makes SPT classification possible.

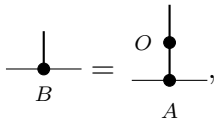
Here we only consider the one-dimensional case; for generalization to higher dimensions see ,e.g., Section 3.3.

2.9.1 Gapped phases in one dimension

Without symmetries, in case of a unique ground state, it is known to be only one phase in one dimension. If considering also degenerate ground-space, then the different phases

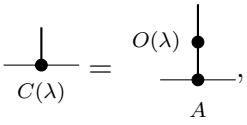
are exactly the different degeneracies. Let us recover this result with the help of MPS. We follow Refs. [22] and [23].

First note that if H and H' are local, gapped Hamiltonians with the same ground-space, then the Hamiltonian path $\gamma H + (1-\gamma)H'$ interpolates between them. Therefore, any parent Hamiltonian of a given state is in the same phase. Consider now two MPS which are defined by tensors A and B satisfying



(2.38)

where O id an invertible operator. Then the path $O(\lambda) = \lambda \cdot \mathrm{Id} + (1-\lambda)\cdot O$ is a continuous path of operators between O and Id. This path is typically invertible. If accidental zero eigenvalue arises, this degeneracy can be lifted by adding another term to it. Therefore, the MPS defined by tensors B and A are connected with a continuous path where the interpolating MPS are described by tensors



(2.39)

where $O(\lambda)$ is invertible. Then the parent Hamiltonian corresponding to the tensor $C(\lambda)$ is a continuous path of local gapped Hamiltonians interpolating between the two endpoints.

To interpolate between different bond dimensions, notice that with the above, one can suppose that the two states are $|\omega_D\rangle$ and $|\omega_d\rangle$, where

$$|\omega_D\rangle = \frac{1}{\sqrt{D}} \sum_{i=1}^{D} |ii\rangle.$$

The reason is that any injective MPS can be transformed with SLOCC to this form, and thus these states are in the same phase as the original MPS. To interpolate between these states, consider the Hamiltonian defined by the terms

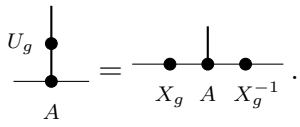
$$h_\lambda = \mathrm{Id} - |\phi_\lambda\rangle\langle\phi_\lambda|,$$

where $|\phi_\lambda\rangle = \lambda|\omega_d\rangle + (1-\lambda)|\omega_D\rangle$. This defines a continuous path of commuting Hamiltonians with unique ground states that interpolate between the two parent Hamiltonians. As the Hamiltonian is a sum of commuting projectors, it is automatically gapped.

Finally, any non-injective MPS – after blocking – is a sum of locally orthogonal injective MPS. Due to the local orthogonality of the different components, the interpolation can be done in parallel in the different sectors.

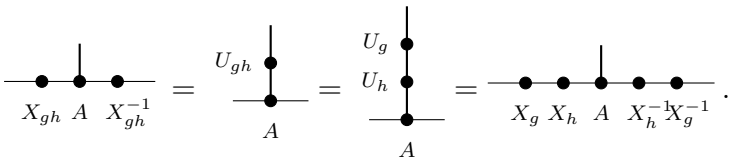
2.9.2 SPT phases in one dimension

At the heart of the classification of SPT phases with MPS lies the Fundamental Theorem. Suppose a phase is protected with on-site symmetries U_g that form a group G. Then, as the ground state is symmetric (in case of unique ground state), the Fundamental Theorem implies



(2.40)

Let us apply first the symmetry U_h and then the symmetry U_g. Then



The gauges on the r.h.s. are unique up to a multiplicative constant. That is, the gauges X_g form a projective representation of the group G:

$$X_g X_g = \omega(g,h) X_{gh}.$$

Given a finite group G, there is a finite number of essentially different projective representations and they form a group (by taking the tensor product). This group is the second cohomology group $H^2(G, \mathbb{C}^*)$. The different SPT phases then correspond to the different projective representations emerging at the virtual level and thus they are labeled by the second cohomology group [22, 23].

Chapter 3

Publications

During my thesis, I worked on several aspects of Tensor Networks. This Chapter contains the reprints of my publications summarizing these projects.

As TNS such as MPS and PEPS are widely used as variational ansatzes in numerical algorithms, it is crucial to understand how well they can approximate Gibbs and ground states of Hamiltonians. In Section 3.1 we show that Gibbs states of local Hamiltonians – and thus ground states of gapped, local Hamiltonians – can be efficiently approximated with PEPS.

Even though this result implicitly gives a polynomial-time algorithm to construct the PEPS approximating such a Gibbs state, calculating expectation values using this representation is hard. In Section 3.2 we provide instead an algorithm to create these states on a quantum computer. Using the quantum computer, measuring expectation values of observables becomes simpler. The algorithm works especially well for commuting Hamiltonians. If the Hamiltonian is also classical, we prove that the algorithm runs exponentially faster than the best known worst-case bound for Monte Carlo algorithms achieving the same goal on a classical computer.

In Section 3.3 we investigate further the states for which our algorithm works. We find that these states share a lot of properties with injective PEPS. In particular, they are unique ground states of their parent Hamiltonians for every finite system size. When these states are defined on a honeycomb lattice, they are actually injective, while this is not the case anymore on the square lattice. We introduce a class of PEPS encompassing these almost injective states and show that many other physically interesting states fall into this class as well. We show when two such PEPS generate the same state, which in turn makes it possible to analyze the symmetries of these states. This result makes the classification of 2D SPT more rigorous.

In Section 3.4 we start investigating local symmetries instead of global ones, such as the gauge symmetries in lattice gauge theories. This required different tools from the previously existing fundamental theorems comparing two TN description of the same state, since in those theorems one assumes invariance under translations.

In Section 3.5 we generalized the fundamental theorem of injective PEPS to any normal non-translationally invariant MPS and PEPS. With this generalization one can readily

investigate local symmetries as in Section 3.4, as well as arbitrary geometries such as higher-dimensional PEPS or states defined on hyperbolic lattices.

In Section 3.6 we then ask how general a fundamental theorem for PEPS can be. We show that there are PEPS tensors for which it is hard (even impossible) to tell whether it generates the zero states for all system sizes or not. This result implies that one can not expect a general fundamental theorem deciding when two PEPS tensors generate the same state.

Finally, in Section 3.7 we use the fundamental theorem developed in Section 3.5 to investigate of entanglement properties of MPS. This new fundamental theorem is required in order to deal with the setting of entanglement theory, which is not translationally invariant.

Each Section in the following contains a short summary of the corresponding publication as well as the reprint of the publication.

3.1 Approximation of Gibbs states with PEPS

This Section contains the publication

- Andras Molnar, Norbert Schuch, Frank Verstraete, and J. Ignacio Cirac. "Approximating Gibbs states of local Hamiltonians efficiently with projected entangled pair states". In: *Phys. Rev. B* 91.4, 045138 (4 Jan. 2015), p. 045138. arXiv: 1406.2973

Tensor Network States provide us with powerful numerical algorithms to explore emergent phenomena in strongly correlated systems. Such algorithms are, for example, the DMRG algorithm [37] widely used in the investigation of one-dimensional systems or the iPEPS algorithm effective for the simulation of certain two-dimensional phenomena [69]. The success of these algorithms suggests that TNS are the right variational ansatz for many-body systems. It is important thus to understand whether that is indeed the case as any variational algorithm based on the wrong ansatz leads to incorrect results.

The goal of this project is therefore to understand how well TNS can perform as variational ansatzes. The usual condensed matter Hamiltonians consist of local interactions, which are often restricted to nearest neighbor ones; one is usually interested in Gibbs and ground states of such Hamiltonians. We would like to approximate these states with TNS such that the approximation results in correct expectation values of every observable (even global ones). This approach makes sure that the energy of the state – the expectation value of the Hamiltonian – is correct. As discussed in Section 2.2, this requirement is equivalent with an approximation in trace norm: we want to find a TNS $\tilde{\rho}$ such that

$$\|\rho - \tilde{\rho}\|_1 \leq \epsilon,$$

where ρ is a Gibbs or ground state of the Hamiltonian. As every state can be exactly represented as TNS [54], see also Section 2.2.1, the relevant question is how many parameters are needed for expressing $\tilde{\rho}$ as TNS. If the number of parameters grow exponentially with the particle number, storing the state on a computer is hopeless for larger system sizes. On the other hand, if the number of parameters required for the approximation grows only polynomially, the state can be stored efficiently on a computer even for larger system sizes. However, note that even for TNS with a polynomial scaling in the bond dimension computing expectation values might still be hard [70].

In this paper, we prove that there exists an operator $\tilde{\rho}$ that can be written as a PEPS with low bond dimension and approximates well the Gibbs state ρ of a local Hamiltonian. We give two approaches for this approximation, one based on the Trotter decomposition of the Gibbs state and the other one based on the cluster expansion of Ref. [56, 57]. We show that the required bond dimension grows only polynomially with the system size. This, in fact, also proves a sub-exponential bound for the ground states of local, gapped Hamiltonians.

Approximating Gibbs states of local Hamiltonians efficiently with PEPS

Andras Molnar,[1] Norbert Schuch,[2] Frank Verstraete,[3] and J. Ignacio Cirac[1]

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[2] *JARA Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany*
[3] *Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria and Department of Physics and Astronomy, Ghent University, Ghent, Belgium*

We analyze the error of approximating Gibbs states of local quantum spin Hamiltonians on lattices with Projected Entangled Pair States (PEPS) as a function of the bond dimension (D), temperature (β^{-1}), and system size (N). First, we introduce a compression method in which the bond dimension scales as $D = e^{O(\log^2(N/\epsilon))}$ if $\beta < O(\log(N))$. Second, building on the work of Hastings[1], we derive a polynomial scaling relation, $D = (N/\epsilon)^{O(\beta)}$. This implies that the manifold of PEPS forms an efficient representation of Gibbs states of local quantum Hamiltonians. From those bounds it also follows that ground states can be approximated with $D = N^{O(\log(N))}$ whenever the density of states only grows polynomially in the system size. All results hold for any spatial dimension of the lattice.

I. INTRODUCTION

Problems dealing with quantum many-body systems in lattices appear very often in different branches of Physics and Chemistry. They typically correspond to discretized versions of first-principle continuum models, like in high-energy physics, atomic physics, or quantum chemistry, or provide a phenomenological description of a complex system, as in condensed matter physics. They are characterized in terms of a lattice Hamiltonian, H, which describes the motion, as well as the interactions among the different constituents. Apart from generating the dynamics via the Schrödinger equation, the Hamiltonian defines the quantum state of the system in thermal equilibrium through the Gibbs density operator,

$$\rho = \frac{e^{-\beta H}}{Z} = \frac{e^{-\beta H}}{\mathrm{tr}\left[e^{-\beta H}\right]}, \tag{1}$$

where Z is the partition function and $\beta = 1/\kappa_B T$ is the inverse temperature (we set the Bolzmann constant $\kappa_B = 1$). This operator encodes all the (statical) physical properties of our systems. Extracting that information becomes a hard problem, even for systems consisting of very few particles. The reason is that, in order to determine expectation values of observables, we have to express ρ in a basis of the corresponding Hilbert space, and the dimension of the latter grows exponentially with the number of lattice sites, N (i.e. volume) of the lattice. This fact is ultimately related to the tensor product structure inherent in quantum mechanical problems dealing with composite objects, and thus ubiquitous in several branches of science.

There exist different ways around that problem, at least in some specific situations. For instance, one can employ sampling techniques in certain models (not suffering from the sign problem), to accurately determine the physical properties of a system in thermal equilibrium. Alternatively, one can restrict oneself to simple tractable families of states depending on few parameters, which can then be determined by variational techniques. This last approach typically requires a good intuition to select which family will encompass all the physical properties that one has to describe, and can easily lead to either wrong or inaccurate results. Yet another approach is that of quantum simulation, where the Hamiltonian of interest is implemented on a different system on which one has enough control[2].

Strictly speaking, the exponential scaling of the dimension of the Hilbert space with the size of the lattice should not be the ultimate reason for the difficulty of quantum many-body problems, at least for the ones that naturally appear in nature. For instance, if H is the sum of terms acting non-trivially only on at most x lattice sites, then we can characterize all possible Hamiltonians with a number of parameters that scales only polynomially with N. If those terms are local, meaning that the distance between the sites on which term of H acts is bounded by a constant, this scale is even linear in N. Thus, for all those problems, ρ itself only depends on few parameters. One says that the states can only explore a very small "corner" of the Hilbert space[3]. Consequently, it may be possible to utilize this fact to find families of states that *describe all possible many-body lattice problems with x-body interactions in thermal equilibrium, and that depend on a number of parameters that only grows polynomially with N*. Thus, a central problem in this context is to find and characterize such a family of states. A first and fundamental step would be to solve that problem for local Hamiltonians, on which we will concentrate in the following.

Matrix Product States (MPS)[4,5] provide the answer for one dimensional models at zero temperature for both, gapped[6,7] and critical models[8]. Specifically, if Ψ_0 is the ground state of such a Hamiltonian there exists a MPS of bond dimension D, Ψ_{MPS}, such that $\|\Psi_0 - \Psi_{\mathrm{MPS}}\| < \epsilon$ with $D = O[poly(N/\epsilon)]$. Note that, in turn, the number of parameters to characterize the MPS scales polynomially with D. This result is strongly connected to the area law[9,10], which is fulfilled (or only slightly violated) for those models and MPS. In higher dimensions and still at zero temperature, it is conjectured (and proven under certain assumptions[11,12]), that the area law still

holds (with logarithmic corrections for certain critical models[13,14]). In that case, one would expect that the Projected Entangled-Pair States (PEPS)[15,16], which extend MPS to higher dimensions, would provide us with the efficient description of that corner of the Hilbert space[3]. Moreover, for any finite temperature (independent of N), an area law has been proven[17] both for Gibbs states (1), as well as for Projected Entangled-Pair Operators (PEPO), the extension of PEPS to mixed sates. This also suggests that PEPOs can efficiently describe Gibbs states of local Hamiltonians. From the physics point of view, this is actually the relevant question, as any extended system can only be cooled down to a certain temperature independent of the system size.

Hasting[1] has already derived some remarkable results addressing that question. He has shown that in d spatial dimensions, one can build a PEPO, ρ_{PEPO}, such that $||\rho - \rho_{\mathrm{PEPO}}||_1 < \epsilon$ with bond dimension scaling as

$$D = e^{O(\beta \log(N/\epsilon)^d)}. \tag{2}$$

This gives a polynomial scaling for one dimension, and a sub-exponential (although superpolynomial) one for higher ones. This result also implies a bound for the approximation of the ground state. In fact, if H is gapped and the density of states for a fixed energy only grows as poly(N), then choosing $\beta = O(\log N)$ in (1) we obtain a state that is as close as we want to the ground state[18]. This means that, under those conditions, we can find a PEPS approximation of the ground state with

$$D = e^{O(\log(N/\epsilon)^{d+1})}. \tag{3}$$

In the present paper we derive the following results. First, we use a novel method to obtain a bound for $\beta \leq O(\log(N))$ independent of the dimension (although still superpolynomial in N),

$$D = e^{O(\log^2(N/\epsilon))}. \tag{4}$$

Under the same condition on the density of states as before, we also obtain that the ground state can be approximated with

$$D = e^{O(\log^2(N/\epsilon))}, \tag{5}$$

independent of the dimension. Finally, using Hastings' construction of the PEPO (see also[19]), we show that it is possible to have a polynomial scaling for any temperature, i.e.

$$D = (N/\epsilon)^{O(\beta)}. \tag{6}$$

The paper is organized as follows. In section II we define the problem we are addressing in this work. Section III derives the bounds (4) and (5) using a technique based on the Trotter expansion. In Section IV we use a different encoding of the PEPO based on Hastings' construction to obtain the polynomial bound (6). In all these sections we quote the results and explain how we have proven them. In the appendix we give details of the proofs.

II. PROBLEM

We consider a growing sequence of finite spin systems, S_n, with two-body interactions. To every system, S_n, we assign a graph, $\mathcal{G}_n = (\mathcal{V}_n, \mathcal{E}_n)$, where the vertices $\mathcal{V}_n$ correspond to the individual spins and the edges $\mathcal{E}_n$ to interactions. The Hamiltonian is such that only the connected points interact:

$$H_n = \sum_{e \in \mathcal{E}_n} h_e, \tag{7}$$

where h_e acts non-trivially on spins v and w if $e = (v, w)$. Even though for simplicity we have considered only nearest neighbor interactions, the results generalize to local more-body interactions. We will assume that the (operator) norm of all the terms in the Hamiltonians is bounded by 1, i.e., $\|h_i\| \leq 1$. If the norm of the Hamiltonians were bounded by J instead of 1, this factor could be included into the definition of the temperature.

We assume that all graphs are connected, and that their degree is uniformly bounded. That is, the number of edges starting from a given point is smaller than some constant z. This implies that $2|\mathcal{E}_n|/z < |\mathcal{V}_n| \leq |\mathcal{E}_n| + 1$. Thus, we can equally characterize the size of the system by the number of spins or interactions, $N = |\mathcal{V}_n|$ and $|\mathcal{E}_n|$, respectively. For convenience we will denote $|\mathcal{E}_n|$ by K and omit the index n in the following.

We also assume that there is a uniformly bounded lattice growth constant. This means that there is a universal constant, γ, such that for any given $e \in E$ and all $l \in \mathbb{Z}^+$

$$\left| \{\mathcal{I} \subseteq \mathcal{E} | \mathcal{I} \text{ connected}, \ e \in \mathcal{I}, \ |\mathcal{I}| = l\} \right| \leq \gamma^l. \tag{8}$$

That is, the number of connected regions having l edges that include a specific edge, e, grows at most exponentially with l. In particular, this is the case if $\mathcal{G}_n$ is a regular lattice in any spatial dimension[20]. Thus, our treatment includes all those cases.

We consider the Gibbs state corresponding to H given by (1). We will construct a PEPO, $\tilde{\rho}$, of bond dimension D, that is close to that state. In particular, for any $\varepsilon > 0$,

$$\left\| e^{-\beta H} - \tilde{\rho} \right\|_1 \leq \varepsilon \|e^{-\beta H}\|_1, \tag{9}$$

where $\|x\|_p = \left[\mathrm{tr}(x^\dagger x)^{p/2}\right]^{1/p}$ stands for the Schatten-p-norm ($\|x\| = \|x\|_\infty$ for the operator norm). We will be interested in how D scales with N (or equivalently, with K) and ε.

By a PEPO on a graph $\mathcal{G} = (\mathcal{E}, \mathcal{V})$ we mean that the operator $\tilde{\rho}$ admits the following form:

$$\tilde{\rho} = \sum_{\alpha: \mathcal{E} \to \{1 \ldots D\}} \bigotimes_{v \in \mathcal{V}} X^v_{\alpha(e^v_1) \ldots \alpha(e^v_{z(v)})}. \tag{10}$$

Here, $X^v_{\alpha(e^v_1) \ldots \alpha(e^v_{z(v)})}$ are operators acting on the vertex v alone, $z(v)$ is the degree of v, and $e^v_1, \ldots e^v_{z(v)}$ are the edges going through v. This definition is the straightforward generalization of PEPS[15] for operators[21,22]. One

can readily see[3] that this operator can be written as a tensor network on the graph $\mathcal{G}$, where the bond dimension is D.

III. CONSTRUCTION BASED ON A TROTTER EXPANSION AND COMPRESSION

In this section we use a Trotter expansion combined with a compression method to approximate the Gibbs state. The intuition about why this expansion should give rise to a PEPO description is the following (see also[23]). Let us assume that the operators h_e commute with each other. Then, the Gibbs state (1) is proportional to a product of exponentials, each of them of the form $e^{-\beta h_e}$. One can easily show that each term in that product creates a link in the PEPO[17]. The bond dimension, D_0, is simply the maximum number of singular values of h_e, when decomposed in terms of the vertices it connects, and thus it is independent of K and the temperature. In the general case where the h_e do not commute with each other, we can still perform a Trotter expansion and approximate ρ (up to a constant factor) by $(\tau^\dagger\tau)^M$ where

$$\tau = \prod_{i=1}^{K} e^{-\beta h_i/2M}. \tag{11}$$

The integer M has to be chosen such that the approximation is good, i.e.

$$\|e^{-\beta H} - (\tau^\dagger\tau)^M\|_1 \leq \varepsilon \|e^{-\beta H}\|_1 \tag{12}$$

for some $\varepsilon > 0$. Now, if we use the same argument we see that each time we apply τ, we create a bond between each pair of vertices that are connected in the graph. That is, we multiply the bond dimension by D_0. Thus, naively, the final bond dimension will be D_0^{2M}, and since M has to grow polynomially with K, we get a very bad bound. However, for large M each of the terms in τ is close to the identity operator. Thus, this operator creates very little entanglement and it should be possible to compress the information that is contained in the bond variables for any pair of connected vertices, and therefore to decrease the bond dimension. In fact, in the case of commuting Hamiltonians one can reduce it to D_0, independent of M. This is, in fact, what we do in this section: we first find M such that (12) holds, and then we compress the bond to get a better scaling of the bond dimension with K.

More specifically, we write $e^{-\beta h_i/2M} = \mathbb{1} + (e^{-\beta h_i/2M} - \mathbb{1})$, then, after collecting the K terms of τ and $\tau^\dagger$ into one product of $2K$ terms, we obtain

$$(\tau^\dagger\tau)^M = \prod_{j=1}^{M}\prod_{i=1}^{2K} e^{-\beta \tilde{h}_i/2M} = \prod_{j=1}^{M}\prod_{i=1}^{2K}(1+x_i), \tag{13}$$

where $\tilde{h_i}$ denotes h_{K+1-i} if $i \leq K$, and h_{i-K} otherwise, and $x_i = e^{-\beta\tilde{h}_i/2M} - \mathbb{1}$. After expanding the product, this operator takes the form

$$(\tau^\dagger\tau)^M = \sum_{\lambda\in\mathcal{M}^b_{M,2K}} \prod_{j=1}^{M}\prod_{i=1}^{2K} x_i^{\lambda_{i,j}}. \tag{14}$$

The sum runs over all $M \times 2K$ matrices with entries 0 or 1, denoted by $\mathcal{M}^b_{M,2K}$. From this sum we only keep those terms in which any given x_i appears at most L times in (14). In Section III B we show that the resulting operator $\tilde{\rho}$ is a good approximation to $(\tau^\dagger\tau)^M$ if $L \approx \log K$.

In section III C we show then that the resulting operator can be written as a PEPO, in the sense of (10), with bond dimension $M^{O(L)}$. The reason why this operator admits a PEPO form can be understood as follows. First we identify each particular term in the expansion of $(\tau^\dagger\tau)^M$ with the help of indices defined on the edges. This can be done by specifying at every edge, i, the position where x_{K+1-i} and/or x_{K+i} appear out of the M possibilities. Once a term is identified, we proceed with the Schmidt decomposition of that term in order to build the local operators $X^v_{\alpha(e_1^v)\ldots\alpha(e^v_{z(v)})}$. Let us notice that the latter only depends on the order in which the operators $x_{e_1^v}$, $x_{e_2^v}$, ... $x_{e^v_{z(v)}}$ appear in the given term, where $e_1^v, \ldots e^v_{z(v)}$ are the edges starting from point v. This order can be obtained locally from the edges that surround v, which contain information about the x involved in each of them. As a result of that, at every edge we have to specify $\binom{M}{L}^2 \approx M^{2L}$ natural numbers. As $M = poly(K)$ and $L = O(\log K)$, this gives a bond dimension $K^{O(\log K)}$ for the approximating operator. Therefore, as $N \leq 2K/z$, we obtain a bond dimension that scales like $N^{O(\log N)}$.

A. Trotter expansion

We know that $(\tau^\dagger\tau)^M$ (τ as in equation (11)) tends to $e^{-\beta H}$ if $M \to \infty$. The question is how big M has to be chosen such that we obtain a good approximation in one-norm. Here we prove that setting $M = poly(K)$ is enough (see also[24]).

We present the proof in two steps. First we show that $\|e^{-\beta H} - (\tau^\dagger\tau)^M\|_1$ is small compared to $\|e^{-\beta H}\|_1$ as long as $\|\eta - \tau\|_{2M}$ is small compared to $\|\eta\|_{2M}$ where $\eta = e^{-\beta H/2M}$. Second, we show that $\|\eta - \tau\|_{2M}$ is small compared to $\|e^{-\beta H/2M}\|_{2M}$. The key point is that both $e^{-\beta H}$ and $(\tau^\dagger\tau)$ are close to $(\mathbb{1} - \beta H/M)^M$. We state the first step as a proposition:

Proposition 1. *If $\varepsilon < 1/3$ and*

$$\|\eta - \tau\|_{2M} \leq \frac{\varepsilon}{M}\|\eta\|_{2M}, \tag{15}$$

then

$$\|\eta^{2M} - (\tau^\dagger\tau)^M\|_1 \leq 9\varepsilon\|\eta^{2M}\|_1. \tag{16}$$

The proof combines the identity $a^m - b^m = \sum_i a^i(a-b)b^{m-i-1}$ with the Hölder inequality for matrices[25] and

it is presented in the Appendix. We state the second statement (that η is close to τ) as a lemma.

Lemma 1. *If $M > 36\beta^2K^2/\epsilon$ and $\epsilon < 1$, then*

$$\|\eta - \tau\|_{2M} \leq \frac{\epsilon}{M}\|\eta\|_{2M}.$$

The main idea is that it is enough to prove the statement for the operator norm, as $\|\eta-\tau\|_{2M}$ is bounded by the Hölder inequality

$$\|\eta - \tau\|_{2M} = \|\eta^{-1}\eta(\eta - \tau)\|_{2M} \leq \|\eta^{-1}\|\|\eta\|_{2M}\|\eta - \tau\|,$$

and $\|\eta^{-1}\|$ is not too big as η is close to the identity operator. In order to show that $\|\eta-\tau\|$ is close to zero, by a simple series expansion we obtain that $\|\eta-\mathbb{1}+\beta H/M\|$ is small and so is $\|\tau - \mathbb{1} + \beta H/M\|$. The statement then follows from the triangle inequality. The detailed proof is presented in the appendix.

Putting together Proposition (1) and Lemma (1), we obtain that the Trotter approximation is ε-close (in one-norm) if the trotter steps are chosen to be $M > 360\beta^2K^2/\varepsilon$.

B. Compression

We approximate now $(\tau^\dagger\tau)^M$ by an operator $\tilde{\rho}$ starting from Eq. (14). This expansion can be pictured as follows. We can think of the resulting operator as a sum:

$$(\tau^\dagger\tau)^M = \sum_{\text{all fillings}}$$

	x_1	x_2	$\dots$	x_{2K}
1	X			
2			X	
$\vdots$		X		
M	X			X

, (17)

where the table can be understood as follows. We begin to read from the upper-left corner, from left to right, row-by-row. Whenever we meet an X in the actual cell, we write down the corresponding operator x_i (according to the column), and otherwise the identity operator. The value assigned to a given table is then the product of those operators. We finally have to sum up the resulting operators for all possible fillings of the table.

The approximating operator $\tilde{\rho}$ can be thought of in the same way, just limiting the number of X's in each of the columns.

$$\tilde{\rho} = \sum_{\substack{\text{filling per} \\ \text{column} \leq L}}$$

	x_1	x_2	$\dots$	x_{2K}
1	X			
2			X	
$\vdots$		X		
M	X			X

. (18)

We want to prove that this is a good approximation: $\|(\tau^\dagger\tau)^M - \tilde{\rho}\|_1 \leq \varepsilon\|\rho\|_1$ if the maximal number of X's per column, L, is chosen big enough. We will show that $L = O(\log K)$ is enough.

Let us first explain the main idea of the proof. Given a set of columns $\mathcal{I} \subseteq \{1, 2 \dots K\}$, define $S(\mathcal{I})$ to be the sum of all tables containing more than L X's in all columns $i \in \mathcal{I}$, but with no restriction for the columns not belonging to $\mathcal{I}$. Formally, let $\mathcal{Q}(\mathcal{I})$ denote the set of these tables:

$$\mathcal{Q}(\mathcal{I}) = \left\{ \lambda \in \mathcal{M}^b_{M,2K} \mid i \in \mathcal{I} \Rightarrow \sum_j \lambda_{i,j} > L \right\},$$

then $S(\mathcal{I})$ is the sum

$$S(\mathcal{I}) = \sum_{\lambda \in \mathcal{Q}(\mathcal{I})} \prod_{j=1}^{M} \prod_{i=1}^{2K} x_i^{\lambda_{i,j}}. \tag{19}$$

In any column that has no restriction, the sum can be evaluated, giving back $e^{-\beta\tilde{h}_i/2M}$ in every row of that column. By evaluating those sums we arrive to a sum containing only a few terms. In these remaining terms still a large number of X's appear, therefore the norm of each such term is small. Thus the one-norm of $S(\mathcal{I})$ can be bounded. We will express $\tilde{\rho}$ with the help of the sums $S(\mathcal{I})$ in order to be able to bound its norm.

We use this observation in order to upper bound the one-norm of $(\tau^\dagger\tau)^M - \tilde{\rho}$. That difference contains one or more columns where there are more than L appearances of X. We regroup the tables as follows. First, given a set of columns, $\mathcal{I}$, we sum up all tables that have more than L appearances of X in the columns $i \in \mathcal{I}$, albeit at most L in all columns $i \notin \mathcal{I}$. This set of tables is the following set:

$$\mathcal{T}(\mathcal{I}) = \left\{ \lambda \in \mathcal{M}^b_{M,2K} \mid \sum_j \lambda_{i,j} > L \Leftrightarrow i \in \mathcal{I} \right\}.$$

The sum of these tables will be called $R(\mathcal{I})$:

$$R(\mathcal{I}) = \sum_{\lambda \in \mathcal{T}(\mathcal{I})} \prod_{j=1}^{M} \prod_{i=1}^{2K} x_i^{\lambda_{i,j}}. \tag{20}$$

Note that the operator $\tilde{\rho}$ is expressed by $R(\emptyset)$, as $\tilde{\rho}$ is the sum of tables that in each column contain at most L X's.

We can express the sum $S(\mathcal{I})$ with the help of $R(\mathcal{I})$:

$$S(\mathcal{I}) = \sum_{\mathcal{J} \supseteq \mathcal{I}} R(\mathcal{J}), \tag{21}$$

because in any table in $S(\mathcal{I})$, the columns containing more than L X's form a set $\mathcal{J} \supseteq \mathcal{I}$. Note that $(\tau^\dagger\tau)^M = S(\emptyset)$, as $(\tau^\dagger\tau)^M$ contains all tables, with no restriction on the number of X's in any column.

The difference $(\tau^\dagger\tau)^M - \tilde{\rho}$ is then

$$(\tau^\dagger\tau)^M - \tilde{\rho} = S(\emptyset) - R(\emptyset). \tag{22}$$

To bound the norm of this difference, we need to express $R(\emptyset)$ with the help of the $S(\mathcal{I})$'s; that is, we need the inverse relation of Eq. (21). This inverse relation is given by the Möbius inversion formula, which is used, for example, in the context of the Kirkwood-Salzburg equations, for a cluster expansion for the partition function[26,27]. The statement of the Möbius inversion is the following.

Let $\mathcal{A}$ be a finite set, $\mathcal{P}(\mathcal{A})$ the set of all its subsets, and V a vector space. Given a function, $f : \mathcal{P}(\mathcal{A}) \to V$, we define the following transformations:

$$\hat{f}(\mathcal{I}) := \sum_{\mathcal{J}:\mathcal{A}\supseteq\mathcal{J}\supseteq\mathcal{I}} f(\mathcal{J}) \tag{23}$$

$$\check{f}(\mathcal{I}) := \sum_{\mathcal{J}:\mathcal{A}\supseteq\mathcal{J}\supseteq\mathcal{I}} (-1)^{|\mathcal{J}\setminus\mathcal{I}|} f(\mathcal{J}). \tag{24}$$

Lemma 2 (Möbius inversion)**.**

$$\hat{\check{f}} = \check{\hat{f}} = f$$

This lemma just expresses that the second transformation is the inverse of the first one. The proof is presented in the Appendix. We will use the lemma by setting $\mathcal{A}$ to be the set of columns, and $f = R$. Thus, comparing the definitions (21) and (23) we deduce that $\hat{f} = S$. Applying the lemma we obtain the desired relation

$$R(\emptyset) = \sum_{\mathcal{I}} (-1)^{|\mathcal{I}|} S(\mathcal{I}),$$

and thus substituting back to Eq. (22)

$$(\tau^\dagger\tau)^M - \tilde{\rho} = S(\emptyset) - \sum_{\mathcal{I}} (-1)^{|\mathcal{I}|} S(\mathcal{I}), \tag{25}$$

therefore

$$(\tau^\dagger\tau)^M - \tilde{\rho} = -\sum_{\mathcal{I}\neq\emptyset} (-1)^{|\mathcal{I}|} S(\mathcal{I}). \tag{26}$$

The one-norm of the difference can be bounded by the triangle inequality:

$$\|(\tau^\dagger\tau)^M - \tilde{\rho}\|_1 \leq \sum_{m=1}^{2K} \binom{2K}{m} \max_{\mathcal{I}:|\mathcal{I}|=m} \|S(\mathcal{I})\|_1. \tag{27}$$

We obtained this form by counting the number of subsets $\mathcal{I}$ of the $2K$ columns that have $|\mathcal{I}| = m$. Now, we need to bound the one-norm of $S(\mathcal{I})$. First of all, as noted before, we can sum up over all indices possessing no restriction. That is, over all $\lambda_{i,j}$ with $i \notin \mathcal{I}$. For example, if $2 \notin \mathcal{I}$ then

$$S(\mathcal{I}) = \sum_{\substack{\text{filling} \leq L \\ \text{for column } i\in\mathcal{I}}} \begin{array}{|c||c|c|c|c|}\hline & x_1 & x_2 & \dots & x_{2K} \\ \hline\hline 1 & X & e^{-\beta h_2} & & \\ \hline 2 & & e^{-\beta h_2} & X & \\ \hline \vdots & & e^{-\beta h_2} & & \\ \hline M & X & e^{-\beta h_2} & & X \\ \hline\end{array}, \tag{28}$$

where we have already summed up for all $\lambda_{2,j}$. Let μ be such a term in $S(\mathcal{I})$ in which each x_i ($i \in \mathcal{I}$) is appearing exactly $k_i > L$ times. The one-norm of this term is bounded by the following lemma.

Lemma 3. *If $M > 72\beta^2K^2$, then*

$$\|\mu\|_1 \leq 3\|e^{-\beta H}\|_1 \left(\frac{3\beta}{M}\right)^{k_1+\dots k_m}.$$

This bound is the consequence of the fact that the x_i's, whose norm is small, appear exactly $k_1+k_2+\dots k_m$ times in μ, while the rest of the operators, that is, $e^{-\beta\tilde{h}_i}$, give almost a Trotter approximation of $e^{-\beta H}$. The proof is presented in Appendix D. The number of such terms μ is given by

$$\binom{M}{k_1}\binom{M}{k_2}\dots\binom{M}{k_m}, \tag{29}$$

as at each column $i \in \mathcal{I}$ one has to choose k_i rows out of the total number of M rows to place the appearing x_i's. Thus the one-norm of $S(\mathcal{I})$ is bounded by the following sum:

$$S(\mathcal{I}) \geq \sum_{k_1>L} \cdots \sum_{k_m>L} 3\|e^{-\beta H}\|_1 \prod_{i=1}^{m} \binom{M}{k_i} \left(\frac{3\beta}{M}\right)^{k_i}, \tag{30}$$

therefore

$$\|S(\mathcal{I})\| \leq 3\|e^{-\beta H}\|_1 \left(\sum_{k>L} \binom{M}{k} \left(\frac{3\beta}{M}\right)^k\right)^m. \tag{31}$$

The sum in the parenthesis can be upper bounded by

$$\sum_{k>L} \binom{M}{k} \left(\frac{3\beta}{M}\right)^k \leq e^{3\beta} \left(\frac{3e\beta}{L}\right)^L$$

(see Lemma 5 in Appendix E) and thus

$$\|S(\mathcal{I})\| \leq 3\|e^{-\beta H}\|_1 \left[e^{3\beta} \left(\frac{3e\beta}{L}\right)^L\right]^m. \tag{32}$$

Substituting the obtained bound into Eq. (27) the following holds for the error of the compression:

$$\|(\tau^\dagger\tau)^M - \tilde{\rho}\|_1 \leq 3\|e^{-\beta H}\|_1 \sum_{m=1}^{2K} \binom{2K}{m} \left[e^{3\beta} \left(\frac{3e\beta}{L}\right)^L\right]^m. \tag{33}$$

Thus, after evaluating the sum, we obtain

$$\left\|(\tau^\dagger\tau)^M - \tilde{\rho}\right\|_1 \leq 3\|e^{-\beta H}\|_1 \left(\left[1 + e^{3\beta} \left(\frac{3e\beta}{L}\right)^L\right]^{2K} - 1\right). \tag{34}$$

As $(1+x/K)^K \leq e^x \leq 1+2x$ as long as $x < 1$, this yields the bound

$$\|(\tau^\dagger\tau)^M - \tilde{\rho}\|_1 \leq 12\|e^{-\beta H}\|_1 K e^{3\beta} \left(\frac{3e\beta}{L}\right)^L. \tag{35}$$

Therefore, if $\beta \leq b \log K$, setting $L = O(\log K/\epsilon)$ implies

$$\|(\tau^\dagger \tau)^M - \tilde{\rho}\|_1 \leq \epsilon \|e^{-\beta H}\|_1, \tag{36}$$

thus the error of the compression is bounded by ϵ if $L = O(\log K/\epsilon)$ and $M > 72\beta^2 K^2$.

C. Coding as a PEPO

We show that the resulting operator $\tilde{\rho}$ admits a PEPO form as in equation (10):

$$\tilde{\rho} = \sum_{\alpha:\mathcal{E}\to\{1\ldots D\}} \bigotimes_{v\in\mathcal{V}} X^v_{\alpha(e_1^v)\ldots\alpha(e^v_{z(v)})}. \tag{37}$$

First, let us consider the Schmidt decomposition of the operators x_i.

$$x_i = e^{-\beta \tilde{h}_i/2M} - 1 = \sum_{\nu=1}^{s} A_\nu^{v,i} \otimes A_\nu^{w,i}, \tag{38}$$

with s being at most d_{phys}^2, where d_{phys} is the dimension of the Hilbert space describing the individual spins, and the edge corresponding to column i is composed of the two particles v and w. Note that there are two columns associated to a Hamiltonian term h_i, $K+1-i$ and $K+i$.

After this decomposition, we can think of $\tilde{\rho}$ as the following sum:

$$\tilde{\rho} = \sum_{\substack{\text{filling per}\\ \text{column} \leq L}} \begin{array}{|c||c|c|c|c|}\hline & x_1 & x_2 & \ldots & x_{2K} \\ \hline\hline 1 & 3 & 1 & 0 & 0 \\ \hline 2 & 0 & 0 & 3 & 0 \\ \hline \vdots & 0 & 3 & 0 & 4 \\ \hline M & 2 & 0 & s & 0 \\ \hline \end{array}, \tag{39}$$

where the sum runs over all fillings that have at most L cells different from 0 in every column. The table means the following. We begin to read the table from left to right, row-by-row. Whenever we meet a cell in column i containing the number k we write down the operator $A_k^{v,i} \otimes A_k^{w,i}$ as in Eq. (38). Otherwise we write down the identity operator. The value of the table is again the product of these operators.

Every term in the above sum is now a tensor product. The local operator acting on particle v depends only on the columns corresponding to the edges surrounding v. Indeed, operators acting non-trivially on particle v occur only in these columns.

Therefore, the index $\alpha(e)$ at edge e will specify a possible filling of the two columns corresponding to e, and the operator $X^v_{\alpha(e_1^v)\ldots\alpha(e^v_{z(v)})}$ will mean the product of the corresponding Schmidt coefficients.

For a given edge $\alpha(e)$ can take

$$D = \left[\sum_{k\leq L} \binom{M}{k} s^k\right]^2 \leq L^2 (sM)^{2L} \tag{40}$$

different values, as the positions of the non-zero elements and their values are needed to be specified for the two columns corresponding to edge e.

In Section III we have shown that we should set $M > 360\beta^2 K^2/\epsilon$ in order to the Trotter approximation be ϵ-close to the Gibbs state. In Section III B we have seen that one can choose L such that the compressed operator, $\tilde{\rho}$, is ϵ-close to the Trotter expansion. Therefore, by the triangle inequality, for any given ϵ that decreases at most polynomially in the system size, one can approximate the Gibbs state with error ϵ, if the Trotter steps are taken to be $poly(K)$ and the compression, L, to be $O(\log(K))$. Thus, our method gives a PEPO approximation with bond dimension $K^{O(\log(K))}$. As $2K/z \leq N$, this is a PEPO with bond dimension $N^{O(\log(N))}$.

In Section III B we only have supposed that $\beta \leq b \log(K)$, or equivalently, $\beta \leq b \log(N)$. If H is gapped and the density of states for a fixed energy only grows as $poly(N)$, then by setting $\beta = O(\log(N))$, the ground state projector is approximated by the Gibbs state with an error decreasing as $poly(N)$. Therefore, our method also gives an $N^{O(\log(N))}$ bond dimensional PEPO approximation of the ground state projector, and thus an $N^{O(\log(N))}$ bond dimensional PEPS approximation for the ground state (for any prescribed error ϵ that decreases at most as $poly(N)$) under the same condition.

IV. Poly(N) BOND DIMENSIONAL APPROXIMATION

In this section we show that with the help of the cluster expansion technique[1] we can approximate the thermal state by an MPO with $N^{O(\beta)}$ bond dimension. For that, we just have to modify theorem 15 in[19] and introduce a more efficient way of encoding the PEPO. That theorem says that for $\beta < \beta^*$ (β^* is a constant) the density operator can be well approximated with the truncated cluster expansion, where only clusters of size at most $O(\log K)$ (equivalently, $O(\log N)$) are included. By a clever choice of the coding of the PEPO, we show that for that temperature one just needs a $poly(N)$ bond dimension, and then, as in[1], we extend the result to lower (but finite) temperatures.

A. Cluster expansion

Before restating theorem 15 in[19] we need to introduce some notation. Let $\mathcal{E}^* = \cup_{k=0}^{\infty} \mathcal{E}^k$, that is, a word w from $\mathcal{E}^*$ denotes a sequence of edges: $w = (w_1 w_2 \ldots w_k)$. Let h_w denote the product of the Hamiltonian terms corresponding to those edges, $h_w = h_{w_1} h_{w_2} \ldots h_{w_k}$, and let $\text{supp}(w)$ be the set of all edges occurring in w.

Every word's support is a set $\mathcal{I} \subseteq \mathcal{E}$. One can break it into connected components: $\mathcal{I} = \cup_i \mathcal{I}_i$ where the $\mathcal{I}_i$'s are connected, and different components do not contain common points. These connected components are also

called clusters. Then, let $\mathcal{W}_L \subseteq \mathcal{E}^*$ be the set of all words whose support contains only connected components of size at most L. β^* will denote a constant such that $\alpha e^{(2z-1)\beta^*}(e^{\beta^*}-1) < 1$, and

$$\tilde{\rho} = \sum_{w \in \mathcal{W}_L} \frac{(-\beta)^{|w|}}{|w|!} h_w. \tag{41}$$

Theorem 15 in[19] contains the following statement:

Theorem 1. *If $\beta \leq \beta^*$, then*

$$\|e^{-\beta H} - \tilde{\rho}\|_1 \leq \|e^{-\beta H}\|_1 \cdot \left(\exp\left(K\frac{x^L}{1-x}\right) - 1\right) \tag{42}$$

with $x = \gamma e^{(2z-1)\beta}(e^{\beta}-1) < 1$.

Similar to equations (56-58) in[19] one can show that the operator $\tilde{\rho}$ admits the following form:

$$\tilde{\rho} = \sum_{\substack{\mathcal{I} \in \mathcal{C}_L \\ \mathcal{I} = \uplus \mathcal{I}_i}} \prod_i \check{f}(\mathcal{I}_i) \tag{43}$$

where $\mathcal{C}_L$ means the subsets of edges $\mathcal{I}$ that does not contain a connected component of size bigger than L, and the connected components of $\mathcal{I}$ are $\mathcal{I}_i$'s. The operators $\check{f}(\mathcal{I}_i)$ act locally on $\mathcal{I}_i$ and are defined as:

$$\check{f}(\mathcal{I}) = \sum_{\substack{w \in \mathcal{I}^* \\ \mathrm{supp}(w) = \mathcal{I}}} \frac{(-\beta')^{|w|}}{|w|!} h_w \ . \tag{44}$$

We show in Appendix F that $\check{f}(\mathcal{I})$ is the Möbius transform of $f(\mathcal{I}) = e^{-\beta' H(\mathcal{I})}$, with $H(\mathcal{I}) = \sum_{e \in \mathcal{I}} h_e$. This observation makes it easier to show that $\tilde{\rho}$ admits the form (43).

B. Coding

We show in this subsection that the truncated cluster expansion $\tilde{\rho}$ (43) can be written as a PEPO [cf. Eq. (10)]. This operator has a very special form. It is a sum of products of local operators, such that the operator acting on a vertex v only depends on the cluster where v is contained in. Therefore, coding $\tilde{\rho}$ as a PEPO will be carried out in two steps. First, we enumerate all $\mathcal{I} \in \mathcal{C}_L$ subsets of edges with the help of an index $\alpha_1 : \mathcal{E} \to \{1, 2 \dots B_1\}$. This indexing will be such that for any given $v \in \mathcal{V}$ vertex the surrounding edges encode the information in which cluster v is located. Once the cluster $\mathcal{I}_i \ni v$ is identified, the operator $\check{f}(\mathcal{I}_i)$ is written as a PEPO with the help of an index $\alpha_2 : \mathcal{E} \to \{1, 2 \dots B_2\}$. The index α used at the description of the PEPO is then the composition of α_1 and α_2 taking $B_1 B_2$ different values.

a. Identifying the clusters. Let the different values of $\alpha_1(e)$ enumerate all clusters containing e and of size at most L. For a given cluster size l, there are at most γ^l clusters containing e (see Eq. 8), therefore there are at most $L\gamma^L$ such clusters. As $L = O(\log K)$, this means that α_1 takes at most $B_1 \leq poly(K)$ different values. Let us now examine how this indexing is related to the original goal: to enumerate all $\mathcal{I} \in \mathcal{C}_L$ subsets of edges. For any given $\mathcal{I} \in \mathcal{C}_L$ subset one can find the corresponding values $(\alpha_1(e))_{e \in \mathcal{E}}$. However, given an indexing, α_1, it might not correspond to such a subset of edges. The reason is the following. Given an indexing $(\alpha_1(e))_{e \in \mathcal{E}}$, each index means a cluster $\mathcal{I}_e$. The subset $\mathcal{I} \in \mathcal{C}_L$ corresponding to this α_1 is $\cup_e \mathcal{I}_e$, if for any two edges e and f either $\mathcal{I}_e = \mathcal{I}_f$, or the two clusters $\mathcal{I}_e$ and $\mathcal{I}_f$ do not have common point. Therefore the indexing does *not* correspond to an $\mathcal{I} \in \mathcal{C}_L$ subset if and only if there are two edges e and f such that $\alpha_1(e)$ and $\alpha_1(f)$ denote two different, but overlapping clusters. Let us join e and f with a path of edges going in the union of the two clusters $\mathcal{I}_e$ and $\mathcal{I}_f$. Along that path there is a contradiction locally; otherwise, e and f cannot specify contradictory information (see Figure 1). Therefore, if an indexing α_1 does not correspond to a subset of edges, then there is a point $v \in \mathcal{V}$ where it can be detected.

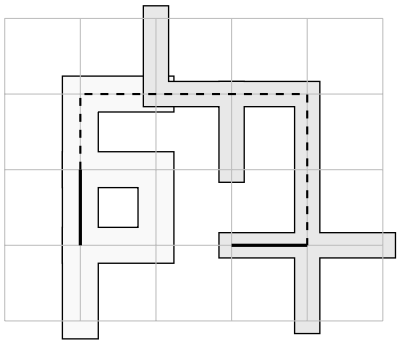

Figure 1. Two clusters specified by the thick edges. The information contained in those edges contradict as the clusters overlap. However, the contradiction appear locally somewhere along the dashed line. Thus, our coding will give the 0 operator for this configuration.

b. Coding the local operators. Any operator defined on at most L particles can be written as a PEPO with bond dimension d_{spin}^{2L}, where d_{spin} is the dimension of the Hilbert space of the particles. For example, an expansion in a product basis of the operators supported on L particles can be viewed as a PEPO. As $\check{f}(\mathcal{I}_i)$ is such a local operator with $L = O(\log K)$, this coding requires an index α_2 with $B_2 = poly(K)$ different values. The local operators used for this construction will be $Y^v_{\alpha_2(e_1^v),\dots\alpha_2(e_{z(v)}^v)}(\mathcal{I}_i)$.

With the help of the index $\alpha = (\alpha_1, \alpha_2)$ the operators $X^v_{\alpha(e_1^v)\dots\alpha(e_{z(v)}^v)}$ are constructed as follows. If $\alpha_1(e_1^v), \alpha_1(e_2^v) \dots \alpha_1(e_{z(v)}^v)$ both specify the same cluster $\mathcal{I}_i$ (or some of them the empty cluster, if compatible with

$\mathcal{I}_i$), then let

$$X^v_{\alpha(e_1^v)\ldots\alpha(e^v_{z(v)})} = Y^v_{\alpha_2(e_1^v),\ldots\alpha_2(e_z^v(v))}(\mathcal{I}_i), \qquad (45)$$

otherwise, if both of them specify the empty cluster, let $X^v_{\alpha(e_1^v)\ldots\alpha(e^v_{z(v)})}$ be $\mathbb{1}$, otherwise let $X^v_{\alpha(e_1^v)\ldots\alpha(e^v_{z(v)})}$ be 0. By construction, the contraction of these tensors really gives $\tilde{\rho}$.

As the index used at the coding, $\alpha = (\alpha_1, \alpha_2)$, can only take $B_1 B_2 = poly(K)$ different values, the above coding is a PEPO with $poly(K)$ (equivalently $poly(N)$) bond dimension. Thus, for any $\beta < \beta^*$, we gave an efficient PEPO description of the Gibbs state. Moreover, Theorem (1) holds for $\beta' = \beta/2M$ instead of β if the trace norm is replaced by $\|.\|_{2M}$ without any essential modification. Therefore, by taking M such that $\beta' < \beta^*$, that is, $M = O(\beta)$, this result can be extended to lower (but finite) temperatures as well (see Proposition 1). However, after this step, the approximating operator will be a PEPO exponentiated M times. Therefore the bond dimension required for the PEPO description of the Gibbs state at arbitrary temperature is $N^{O(\beta)}$.

V. SUMMARY AND OUTLOOK

We have analyzed the ability of tensor networks to describe thermal (Gibbs) equilibrium states of lattice Hamiltonians with local interactions. First, using a Trotter expansion and a compression method, we have shown that it is possible to approximate that state with a PEPO whose bond dimension scales as $N^{O(\log N)}$, where N is the system size (number of vertices in the lattice). This result is valid for any finite temperature and spatial dimension. It also holds true at zero temperature as long as the Hamiltonian is gapped and the density of states for any energy interval only grows polynomially with the system size. Second, building on Hastings' construction[1], we have shown that it is possible to find a PEPO with a $poly(N)$ bond dimension at any finite temperature and spatial dimension.

There are some straightforward implications of the results derived here. First, even though we have concentrated on PEPOs, it is trivial to express our results in terms of (pure) PEPS. At finite temperature, we can just consider the PEPO corresponding to half the temperature, and apply it to locally maximally entangled states in order to obtain a purification in terms of a PEPS with a polynomially growing bond dimension[21]. At zero temperature, we can simply apply the constructed PEPO to a random product state in order to show that there exists a PEPS with $D = N^{O(\log N)}$. Second, for translationally invariant problems in regular lattices, our construction may break translational invariance (as we select some order of the bonds). But it is always possible[5] to make a PEPO (or PEPS) translationally invariant with an increase of the bond dimension by just a factor of N. Third, even though we have considered Hamiltonians interacting along the edges in the graph, our construction can be easily extended to the case in which the local Hamiltonians act on plaquettes. The idea is that at the Trotter decomposition we have made no assumption on the support of the individual Hamiltonian terms, whereas at the coding procedure, we still need to keep information contained in a constant number of columns: in an edge $e = (v, w)$, we can keep the information contained in the columns corresponding to Hamiltonian terms that act non-trivially on either v or w. In such a coding the same piece of information is specified in more than one edge, but their consistency can be checked locally, at the vertices. The cluster expansion technique can be applied with no essential modification as the number of terms acting on the boundary of a cluster can still be upper bounded by a constant times the size of the cluster, and the number of clusters containing l terms is still bounded by γ^l, where γ is a lattice growth constant[20]. Finally, our construction can also be straightforwardly extended to fermions with the result that we just have to use fermionic PEPS[28].

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Appendix A: Proof of Proposition 1

Here we present the proof of Proposition 1. The proof consists of two steps. First, by the positivity of η, we show that if $\varepsilon < 1/3$ and

$$\|\eta - \tau\|_{2M} \leq \frac{\varepsilon}{M}\|\eta\|_{2M}, \qquad (A1)$$

then

$$\|\eta^2 - \tau^\dagger\tau\|_M \leq 3\varepsilon\|\eta^2\|_M. \qquad (A2)$$

Using the identity $a^2 - b^2 = a(a-b) + (a-b)b$ and the triangle inequality we obtain

$$\|\eta^2 - \tau^\dagger\tau\|_M = \|\eta(\eta-\tau)\|_M + \|(\eta-\tau^\dagger)\tau\|_M, \qquad (A3)$$

thus using the Hölder inequality and that $\|X\|_{2M} = \|X^\dagger\|_{2M}$, we conclude that

$$\|\eta^2 - \tau\tau^\dagger\|_M \leq (\|\eta\|_{2M} + \|\tau\|_{2M})\,\|\eta - \tau\|_{2M}. \qquad (A4)$$

$\|\eta - \tau\|_{2M}$ is bounded by the assumptions of the statement, and so is $\|\tau\|_{2M}$ by the triangle inequality. Therefore

$$\|\eta^2 - \tau\tau^\dagger\|_M \leq (2 + \frac{\varepsilon}{M})\frac{\varepsilon}{M}\|\eta\|_{2M}^2. \tag{A5}$$

η is positive, thus $\|\eta\|_{2M}^2 = \|\eta^2\|_M$. If $\varepsilon < 1$, then

$$\|\eta^2 - \tau\tau^\dagger\|_M \leq 3\frac{\varepsilon}{M}\|\eta^2\|_M. \tag{A6}$$

This completes the proof of the first step.

Second, we prove that if Eq. (A6) holds, then

$$\|\eta^{2M} - (\tau^\dagger\tau)^M\|_1 \leq 9\varepsilon\|\eta^{2M}\|_1.$$

The proof is basically the same as that of the first step. Using the identity $a^m - b^m = \sum_i a^i(a-b)b^{m-i-1}$ and the triangle inequality we obtain

$$\|\eta^{2M} - (\tau^\dagger\tau)^M\|_1 \leq \sum_{i=0}^{M-1} \|\eta^{2i}(\eta^2 - \tau^\dagger\tau)(\tau^\dagger\tau)^{M-i-1}\|_1 \tag{A7}$$

Hence by Hölder's inequality the difference is upper bounded by

$$\sum_{i=0}^{M-1} \left\|\eta^{2i}\right\|_{\frac{M}{i}} \left\|\eta^2 - (\tau^\dagger\tau)\right\|_M \left\|(\tau^\dagger\tau)^{M-i-1}\right\|_{\frac{M}{(M-i-1)}}. \tag{A8}$$

For X positive semidefinite, and any real number r, $X^r \geq 0$, and thus by the definition of the Schatten norms

$$\|X^r\|_{M/r} = \|X\|_M^r. \tag{A9}$$

Applying (A9) to η and $\tau^\dagger\tau$ in (A8), the inequality takes the following form:

$$\|\eta^{2M} - (\tau^\dagger\tau)^M\|_1 \leq \sum_{i=0}^{M-1} \|\eta^2\|_M^i \|\eta^2 - \tau^\dagger\tau\|_M \|\tau^\dagger\tau\|_M^{M-i-1} \tag{A10}$$

$\|\eta^2 - \tau^\dagger\tau\|_M$ is bounded by Eq. (A6). Hence, by the triangle inequality, $\|\tau^\dagger\tau\|_M$ is bounded as well,

$$\|\tau^\dagger\tau\|_M \leq \|\eta^2\|_M + \|\eta^2 - \tau^\dagger\tau\|_M \leq \left(1 + \frac{3\varepsilon}{M}\right)\|\eta^2\|_M.$$

As $1 + 3\varepsilon/M > 1$, we can upper bound the sum by taking $(1 + 3\varepsilon/M)^M$ as common factor in every term,

$$\|\eta^{2M} - (\tau^\dagger\tau)^M\|_1 \leq M\frac{\varepsilon}{M}\left(1 + \frac{3\varepsilon}{M}\right)^M \|\eta^2\|_M^M. \tag{A11}$$

Since $(1 + 3\varepsilon/M)^M < e^{3\varepsilon} < 3$, if $\epsilon \leq 1/3$, the statement of the Proposition follows:

$$\|\rho^{2M} - (\tau^\dagger\tau)^M\|_1 \leq 9\varepsilon\|\eta^2\|_M^M. \tag{A12}$$

Appendix B: Proof of lemma 1

Here we present the proof of Lemma 1, and derive how big the number of Trotter steps should be chosen for a good approximation of the Gibbs state. The proof relies on the fact that if M is big enough, then both η and τ are close to $\mathbb{1} - \beta H/2M$.

By the use of Hölder's inequality we obtain

$$\|\eta - \tau\|_{2M} = \|\eta^{-1}\eta(\eta - \tau)\|_{2M} \leq \|\eta\|_{2M}\|\eta^{-1}\|\|\eta - \tau\|.$$

The norm of η^{-1} can be upper bounded by a constant if $M > \beta K/2$:

$$\|\eta^{-1}\| \leq e^{\beta K/2M} \leq 3. \tag{B1}$$

The norm of $\eta - \tau$ will be bounded with the help of the triangle inequality, by adding and subtracting $\mathbb{1} - \beta H/2M$:

$$\|\eta - \tau\| \leq \left\|\eta - \mathbb{1} + \frac{\beta H}{2M}\right\| + \left\|\tau - \mathbb{1} + \frac{\beta H}{2M}\right\|. \tag{B2}$$

We will use the following bound on the Taylor expansion of the exponential function to upper bound these expressions.

Lemma 4. *The following two bounds hold:*

$$\left\|e^A - \mathrm{Id}\right\| \leq \|A\| e^{\|A\|},$$

$$\left\|e^A - \mathrm{Id} - A\right\| \leq \frac{\|A\|^2}{2}e^{\|A\|}.$$

Proof. $e^A = \sum_n \frac{A^n}{n!}$, thus

$$e^A - \sum_{n=0}^{k} \frac{A^n}{n!} = \sum_{n=k+1}^{\infty} \frac{A^n}{n!}. \tag{B3}$$

Therefore the norm of the difference can be upper bounded by the triangle inequality

$$\|e^A - \sum_{n=0}^{k} \frac{A^n}{n!}\| \leq \sum_{n=k+1}^{\infty} \frac{\|A\|^n}{n!} \leq \frac{\|A\|^{k+1}}{(k+1)!}\sum_{n=0}^{\infty} \frac{\|A\|^n}{n!}, \tag{B4}$$

since $(n+k+1)! \geq n!(k+1)!$. Summing up we have the desired inequality

$$\|e^A - \sum_{n=0}^{k} \frac{A^n}{n!}\| \leq \frac{\|A\|^{k+1}}{k+1!}e^{\|A\|}. \tag{B5}$$

The statements correspond to the particular cases $k = 0, 1$. □

Due to the previous lemma, we can bound the first part of the right hand side of Eq. B2:

$$\left\|e^{-\frac{\beta H}{2M}} - 1 + \frac{\beta H}{2M}\right\| \leq \frac{\beta^2 K^2}{8M^2}e^{\beta K/2M} \leq \frac{\varepsilon}{2M}. \tag{B6}$$

If $M \geq \beta^2 K^2/\epsilon$ and $M \geq \frac{\beta K}{2}$, because then $e^{\beta K/2M} \leq 3$ and $3/8 \leq 1/2$.

The second part of the right hand side of Eq. B2 can be written as

$$\tau - \mathbb{1} + \frac{\beta H}{2M} = \prod_i [\mathbb{1} + x_i] - \mathbb{1} + \frac{\beta H}{2M}, \tag{B7}$$

where x_i is as in Eq. (14). Let us expand the product. The zeroth term cancels out, whereas the 1st order term is

$$\sum_i x_i + \frac{\beta H}{2M}.$$

The norm of the sum of the k^{th} order terms can be upper bounded by

$$\binom{K}{k}\left(\frac{\beta}{2M}e^{\frac{\beta}{2M}}\right)^k \leq \left(\frac{3\beta K}{2M}\right)^k$$

if $M \geq \beta/2$, because there are $\binom{K}{k}$ k^{th} order terms, and the norm of $\|x_i\|$ can be bounded by lemma 4:

$$\|x_i\| \leq \frac{\beta}{2M}e^{\frac{\beta}{2M}}.$$

Therefore, after expanding the product in Eq. (B7), we obtain that

$$\left\|\tau - 1 + \frac{\beta H}{2M}\right\| \leq \left\|\sum_i x_i + \frac{\beta h_i}{2M}\right\| + \sum_{k=2}^{\infty}\left(\frac{3K\beta}{2M}\right)^k. \tag{B8}$$

The first term can be again bounded by Lemma 4 as $x_i + \beta h_i/2M = e^{-\beta h_i/2M} - \mathbb{1} + \beta h_i/2M$:

$$\left\|\sum_i x_i - \frac{\beta h_i}{2M}\right\| \leq K\frac{\beta^2}{4M^2}e^{\frac{\beta}{2M}} \leq \frac{K\beta^2}{M^2}, \tag{B9}$$

since if $M > \beta/2$, then $e^{\frac{\beta}{2M}} < 4$. The second term can be upper bounded by

$$\sum_{k=2}^{\infty}\left(\frac{3K\beta}{2M}\right)^k = \left(\frac{3K\beta}{2M}\right)^2 \frac{1}{1-\frac{3K\beta}{2M}} \leq \frac{5K^2\beta^2}{M^2}, \tag{B10}$$

since if $M > 3K\beta$, then $\frac{1}{1-\frac{3K\beta}{2M}} \leq 2$, and $9/2 \leq 5$. Finally, $K > 1$ and thus the sum of the bounds obtained in Eq. (B9) and in Eq. (B10) can be upper bounded by

$$\left\|\tau - 1 + \frac{\beta H}{2M}\right\| \leq \frac{6K^2\beta^2}{M^2} \leq \frac{\varepsilon}{2M}, \tag{B11}$$

if $M > 12K^2\beta^2\frac{1}{\varepsilon}$.

Putting together the two bounds in Eq. (B6) and Eq. (B11), we obtain that

$$\|\eta - \tau\| \leq \frac{\epsilon}{M} \tag{B12}$$

if $M > 12K^2\beta^2/\varepsilon$. Therefore, the statement follows: if $M > 36K^2\beta^2/\varepsilon$, then

$$\|\eta - \tau\|_{2M} \leq \frac{\epsilon}{M}\|\eta\|_{2M}. \tag{B13}$$

Appendix C: Proof of the Möbius inversion

Here we prove the Lemma 2. The first part of the statement is that $\check{\hat{f}} = f$. Let us define $f'(I)$ as

$$f'(\mathcal{I}) = \sum_{\mathcal{J}\supseteq\mathcal{I}}(-1)^{|\mathcal{J}\setminus\mathcal{I}|}\hat{f}(\mathcal{J}). \tag{C1}$$

Then, the statement is that $f'(\mathcal{I}) = f(\mathcal{I})$. Let us express $\hat{f}$ with the help of f as in Eq. (23):

$$f'(\mathcal{I}) = \sum_{\mathcal{J}\supseteq\mathcal{I}}(-1)^{|\mathcal{J}\setminus\mathcal{I}|}\sum_{\mathcal{K}\supseteq\mathcal{J}} f(\mathcal{K}). \tag{C2}$$

By changing the order of the sums we obtain

$$f'(\mathcal{I}) = \sum_{\mathcal{K}\supseteq\mathcal{I}} f(\mathcal{K}) \sum_{\mathcal{J}:\mathcal{K}\supseteq\mathcal{J}\supseteq\mathcal{I}}(-1)^{|\mathcal{J}\setminus\mathcal{I}|}. \tag{C3}$$

We evaluate now the second sum. Suppose first $\mathcal{K} \neq \mathcal{I}$: then

$$\sum_{\mathcal{J}:\mathcal{K}\supseteq\mathcal{J}\supseteq\mathcal{I}}(-1)^{|\mathcal{J}\setminus\mathcal{I}|} = \sum_{\mathcal{J}'\subseteq\mathcal{K}\setminus\mathcal{I}}(-1)^{|\mathcal{J}'|} = (1-1)^{|\mathcal{K}\setminus\mathcal{I}|} = 0.$$

Otherwise, if $\mathcal{K} = \mathcal{I}$, then the sum is one. Substituting this back in the expression of $f'(\mathcal{I})$, we get

$$f'(\mathcal{I}) = \sum_{\mathcal{K}\supseteq\mathcal{I}} f(\mathcal{K}) \sum_{\mathcal{J}:\mathcal{K}\supseteq\mathcal{J}\supseteq\mathcal{I}}(-1)^{|\mathcal{J}\setminus\mathcal{I}|} = f(\mathcal{I}). \tag{C4}$$

This proves the first part of the statement. The second part, $\hat{\check{f}} = f$, works similarly. Let us define now f'' as follows:

$$f''(\mathcal{I}) = \sum_{\mathcal{J}\subseteq\mathcal{I}}\check{f}(\mathcal{J}). \tag{C5}$$

Thus, we have to prove that $f'' = f$. Substituting back the expression for $\check{f}$ (as in Eq. 24) in this equation, we obtain

$$f''(\mathcal{I}) = \sum_{\mathcal{J}\subseteq\mathcal{I}}\sum_{\mathcal{K}\subseteq\mathcal{J}}(-1)^{|\mathcal{J}\setminus\mathcal{K}|}f(\mathcal{K}). \tag{C6}$$

By changing the order of the two sums we obtain

$$f''(\mathcal{I}) = \sum_{\mathcal{K}\subseteq\mathcal{I}} f(\mathcal{K}) \sum_{\mathcal{J}:\mathcal{K}\subseteq\mathcal{J}\subseteq\mathcal{I}}(-1)^{|\mathcal{J}\setminus\mathcal{K}|}. \tag{C7}$$

The second sum is again $\delta_{\mathcal{K},\mathcal{I}}$, and thus

$$f''(\mathcal{I}) = f(\mathcal{I}). \tag{C8}$$

Appendix D: Proof of Lemma 3

Here we present the proof of Lemma 3. In μ two types of terms occur. First, if i refers to a column that has been summed up ($i \notin \mathcal{I}$), then in every row of that column

the term $e^{-\beta\tilde{h}_i}$ appears. Second, if $i \in \mathcal{I}$, then the sum on that column has not been evaluated, therefore the corresponding term in row j is $x_i^{\lambda_{i,j}}$. We now separate these terms:

$$\mu = \prod_{j=1}^{M} \prod_{i\in\mathcal{I}} y_i^{\lambda_{i,j}} \prod_{i\in\{1..2K\}} e^{-\beta\tilde{h}_i/2M}, \tag{D1}$$

where we have introduced

$$y_i = \prod_{j<i} e^{-\beta\tilde{h}_j/2M} x_i \prod_{j<i} e^{\beta\tilde{h}_j/2M} \cdot e^{\beta\tilde{h}_i/2M}. \tag{D2}$$

The norm of y_i can be bounded by the norm of x_i as follows:

$$\|y_i\| \le \|x_i\| e^{\beta K/M} \tag{D3}$$

because $\|e^{-\beta\tilde{h}_j/2M}\| \le 1$ and $\|e^{\beta\tilde{h}_i/2M}\| \le e^{\beta/2M}$ and there are at most $2K$ such terms in y_i. Thus, by applying Lemma 4 to x_i, we obtain:

$$\|y_i\| \le \|x_i\| e^{\beta K/M} \le \frac{\beta}{2M} e^{\beta/2M} e^{\beta K/M} \le \frac{3\beta}{2M}, \tag{D4}$$

since $e^{\beta(2K+1)/2M} \le 3$ if $M > 2\beta K > \beta(K+1/2)$. We now apply Hölder's inequality to Eq. (D1) in order to bound $\|\mu\|_1$:

$$\|\mu\|_1 \le \prod_i \|y_i\|^{\sum_j \lambda_{i,j}} \left\| \prod_{i\in\{1..2K\}} e^{-\beta\tilde{h}_i/2M} \right\|_M^M.$$

The last expression of the right hand side is $(\tau^\dagger\tau)$ from the Trotter expansion formula. By the use of an other Hölder's inequality

$$\|\tau^\dagger\tau\|_M \le \|\tau\|_{2M}^2.$$

Using the triangle inequality and Lemma 1 with the choice $\epsilon = 1/2$, we obtain that

$$\|\tau\|_{2M} \le \left(1 + \frac{1}{2M}\right) \|e^{-\beta H/2M}\|_{2M} \tag{D5}$$

if $M > 72\beta^2K^2$; therefore

$$\|\mu\|_1 \le \prod_i \|y_i\|^{k_i} \left(1 + \frac{1}{2M}\right)^{2M} \|e^{-\beta H/2M}\|_{2M}^{2M}. \tag{D6}$$

Using the bound (D4) on $\|y_i\|$, and the fact that $(1 + 1/2M)^{2M} < e < 3$, we obtain the statement of the lemma,

$$\|\mu\|_1 \le 3 \left(\frac{3\beta}{M}\right)^{k_1+\ldots k_n} \|e^{-\beta H}\|_1. \tag{D7}$$

Appendix E: Lemma on the sum of binomial coefficients

We need the following lemma to upper bound a sum of binomial coefficients in Eq. (31):

Lemma 5. $\sum_{k>L} \binom{M}{k} x^k \le e^{Mx} \left(\frac{eMx}{L}\right)^L$.

Proof. First, as $\binom{M}{k} \le M^k/k!$, we have

$$\sum_{k>L} \binom{M}{k} x^k \le \sum_{k\ge L} \frac{1}{k!} (Mx)^k. \tag{E1}$$

We then use $(L+n)! \ge n!L!$ and sum up over $n = k - L$.

$$\sum_{k\ge L} \binom{M}{k} x^k \le \frac{1}{L!} (Mx)^L e^{Mx}. \tag{E2}$$

Finally, by Stirling's formula, we have the desired result:

$$\sum_{k>L} \binom{M}{k} x^k \le e^{Mx} \left(\frac{eMx}{L}.\right)^L \tag{E3}$$

□

Appendix F: On the cluster expansion

In this Section we show how to use the Möbius inversion to reproduce the cluster expansion. In particular, we show that

$$g(\mathcal{I}) = \sum_{\substack{w\,\in\,\mathcal{I}^* \\ \mathrm{supp}(w)\,=\,\mathcal{I}}} \frac{(-\beta')^{|w|}}{|w|!} h_w \tag{F1}$$

is the (inverse) Möbius transform[29] of

$$f(\mathcal{J}) = e^{-\beta' H(\mathcal{J})}. \tag{F2}$$

Let us consider the Möbius transform of g:

$$\hat{g}(\mathcal{I}) = \sum_{\mathcal{J}\subseteq\mathcal{I}} g(\mathcal{J}) = \sum_{\mathcal{J}\subseteq\mathcal{I}} \sum_{\substack{w\,\in\,\mathcal{J}^* \\ \mathrm{supp}(w)\,=\,\mathcal{J}}} \frac{(-\beta')^{|w|}}{|w|!} h_w. \tag{F3}$$

This means that in $\hat{g}$ we have to sum up for all words in $\mathcal{I}^*$. Indeed, in the sum every word is counted exactly once as we sum up all possible supports. This implies that

$$\hat{g}(\mathcal{I}) = e^{-\beta' H(\mathcal{I})} = f(\mathcal{I}), \tag{F4}$$

and therefore by the Möbius inversion formula $g = \check{f}$.

We now show that obtaining the form Eq. (43) of $\tilde{\rho}$ is much easier with these tools. The proof follows from

the multiplicativity of $\check{f}$: if $\mathcal{I}$ and $\mathcal{J}$ are non-overlapping clusters, then $\check{f}(\mathcal{I}\cup\mathcal{J}) = \check{f}(\mathcal{I})\check{f}(\mathcal{J})$. Indeed,

$$\check{f}(\mathcal{I}\cup\mathcal{J}) = \sum_{\mathcal{K}\subseteq\mathcal{I}\cup\mathcal{J}} (-1)^{|\mathcal{I}\cup\mathcal{J}\setminus\mathcal{K}|} e^{-\beta H(\mathcal{K})}, \tag{F5}$$

where we have used the multiplicativity of the exponential. $\mathcal{K}$ can be broken into two parts: $\mathcal{K}_\mathcal{I} = \mathcal{K}\cap\mathcal{I}$ and $\mathcal{K}_\mathcal{J} = \mathcal{K}\cap\mathcal{J}$. Then both the -1 factor and the exponential factorizes as follows:

$$\check{f}(\mathcal{I}\cup\mathcal{J}) = \sum_{\substack{\mathcal{K}_\mathcal{I}\subseteq\mathcal{I}\\ \mathcal{K}_\mathcal{J}\subseteq\mathcal{J}}} (-1)^{|\mathcal{I}\setminus\mathcal{K}_\mathcal{I}|}(-1)^{|\mathcal{J}\setminus\mathcal{K}_\mathcal{J}|} e^{-\beta H(\mathcal{K}_\mathcal{I})} e^{-\beta H(\mathcal{K}_\mathcal{J})} \tag{F6}$$

and this sum is nothing but $\check{f}(\mathcal{I})\cdot\check{f}(\mathcal{J})$. This implies that the Gibbs state admits the following form:

$$\tilde{\rho} = \sum_{\mathcal{I}\subseteq\mathcal{E}} \prod_{\substack{i\,:\,\mathcal{I}_i \text{ are the}\\ \text{clusters in } \mathcal{I}}} \check{f}(\mathcal{I}_i), \tag{F7}$$

and thus the approximation $\tilde{\rho}$ is nothing but

$$\tilde{\rho} = \sum_{\substack{\mathcal{I}\,\in\,\mathcal{C}_L\\ \mathcal{I}=\uplus\mathcal{I}_i}} \prod_i \check{f}(\mathcal{I}_i). \tag{F8}$$

as in Eq. (43).

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3.2 Rapid adiabatic preparation of injective PEPS and Gibbs states

In this Section, we include the following paper:

- Yimin Ge, András Molnár, and J. Ignacio Cirac. "Rapid Adiabatic Preparation of Injective Projected Entangled Pair States and Gibbs States". In: *Phys. Rev. Lett.* 116.8 (Feb. 2016), arXiv:1508.00570. arXiv: 1508.00570

The previous project provides implicitly a polynomial-time algorithm to prepare a PEPS representation of the Gibbs state of a local Hamiltonian on a classical computer. The obtained representation, however, does not provide the ability to calculate expectation values of local observables: contracting PEPS in general is a hard problem [70]. To gain further insight into thermal states, one thus needs to develop other techniques. Building on Feynman's original proposal, one can use quantum computers to prepare these states. Once the state is represented on a quantum system, measuring expectation values of observables is efficiently feasible.

In this Section, we propose an algorithm to prepare Gibbs states of commuting Hamiltonians on a quantum computer. Since every classical Hamiltonian is commuting, one readily obtains a quantum algorithm that prepares Gibbs states of classical Hamiltonians. Apart from Gibbs states, the algorithm is also suited for the preparation of injective PEPS. We show that for a Hamiltonian consisting of N particles the algorithm requires $O(N\text{polylog}(N/\epsilon))$ gates to prepare a state that is ϵ close to its Gibbs state, provided the Hamiltonian satisfies a uniform gap condition: there is a gapped path consisting of local changes that connects it to a trivial Hamiltonian. For classical Hamiltonians, the number of gates can be compared to the Markov chain Monte Carlo (MCMC) methods, as this condition is the same under which the existence of rapid mixing is usually investigated. For MCMC, the best known worst-case bound for the mixing time (the number of elementary gates expressed with the help of the number of particles) is $O(N^2)$, thus our algorithm scales better. If we allow for parallelization, i.e. we compare the circuit depth of the two algorithms, our algorithm achieves an exponential speedup.

The idea behind the algorithm is simple: we construct a parent Hamiltonian of the state and by slowly interpolating between a trivial Hamiltonian and this parent Hamiltonian, we obtain an adiabatic state preparation protocol. This naive algorithm, however, has very bad worst-case run-time bounds. If the Hamiltonian satisfies a uniform gap condition, then better run-time bounds can be achieved by changing the Hamiltonian terms one by one. Finally, with the help of the Lieb-Robinson bound, we show that these local changes can be replaced by local unitaries further reducing the number of gates.

Rapid Adiabatic Preparation of Injective Projected Entangled Pair States and Gibbs States

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We propose a quantum algorithm for many-body state preparation. It is especially suited for injective projected entangled pair states and thermal states of local commuting Hamiltonians on a lattice. We show that for a uniform gap and sufficiently smooth paths, an adiabatic runtime and circuit depth of $O(\mathrm{polylog}N)$ can be achieved for $O(N)$ spins. This is an almost exponential improvement over previous bounds. The total number of elementary gates scales as $O(N\mathrm{polylog}N)$. This is also faster than the best known upper bound of $O(N^2)$ on the mixing times of Monte Carlo Markov chain algorithms for sampling classical systems in thermal equilibrium.

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Quantum computers are expected to have a deep impact in the simulation of *quantum* many-body systems, as initially envisioned by Feynman [1]. In fact, quantum algorithms have potential applications in diverse branches of science, ranging from condensed matter physics, atom physics, high-energy physics, to quantum chemistry [2]. Lloyd [3] was the first to devise a quantum algorithm to simulate the dynamics generated by few-body interacting Hamiltonians. When combined with the adiabatic theorem [4,5], the resulting algorithms allow one to prepare ground states of local Hamiltonians, and thus to investigate certain quantum many-body systems at zero temperature. Quantum algorithms have also been introduced to prepare so-called projected entangled pair states (PEPS) [6–8], which are believed to approximate ground states of local gapped Hamiltonians. Furthermore, quantum algorithms have also been proposed to sample from Gibbs distributions [9–14], which describe physical systems in thermal equilibrium. The computational time of most of these algorithms is hard to compare with that of their classical counterparts, as it depends on specific (e.g., spectral) properties of the Hamiltonians which are not known beforehand. However, they do not suffer from the sign problem [15], which indicates that they could provide significant speedups.

Quantum computers may also offer advantages in the simulation of *classical* many-body systems. For instance, quantum annealing algorithms [16,17] have been devised to prepare the lowest energy spin configuration of a few-body interacting classical Hamiltonian, which has obvious applications in optimization problems. Quantum algorithms have also been proposed to sample from their Gibbs distributions at finite temperature [18–23]. Apart from applications in classical statistical mechanics, similar problems appear in other areas of intensive research, e.g., machine learning. Speedups as a function of spectral gaps have been analyzed in Refs. [12,21,22]; the scaling with large system sizes, which is of particular interest for applications in deep machine learning [24], is however not optimal.

In this Letter we propose and analyze a quantum algorithm to *efficiently* prepare a particular set of states. This set contains two classes relevant for lattice problems: (i) injective PEPS [25]; (ii) Gibbs states of locally commuting Hamiltonians. Class (ii) contains all classical Hamiltonians, and thus the quantum algorithm allows us to sample Gibbs distributions of classical problems at finite temperature.

Our algorithm outperforms all other currently known algorithms for these two problems in the case that the minimum gap Δ occurring in the adiabatic paths (to be defined below) is lower bounded by a constant. We show that the computational time for a quantum computer, given by the number of elementary gates in a quantum circuit, scales only as

$$T = O(N\mathrm{polylog}(N/\epsilon)), \tag{1}$$

where N is the number of local Hamiltonian terms, ϵ the allowed error in trace distance and the degree of the polynomial depends on the geometry of the lattice. Note that an obvious lower bound on the computational time is $\Omega(N)$, as each of the spins has to be addressed at least once. Thus, Eq. (1) is almost optimal. Furthermore, the algorithm is parallelizable, so that the depth of the circuit becomes

$$D = O(\mathrm{polylog}(N/\epsilon)). \tag{2}$$

This parallelization may also become very natural and relevant in analog quantum simulation, as is the case for atoms in optical lattices [26].

One of the best classical algorithms to sample according to the Gibbs distribution of a general classical Hamiltonian is the well-known Metropolis algorithm [27]. The currently best

upper bound to its computational time is $T = O(N^2/\Delta_{\text{stoch}})$ [28], where Δ_{stoch} is the gap of the generator of the stochastic matrix. We will see that given any stochastic matrix, one can always construct a quantum adiabatic algorithm with the same gap $\Delta = \Delta_{\text{stoch}}$, and thus we obtain a potential quantum speedup of almost a factor of N. Under parallelization, the circuit depth is almost exponentially shorter. Our algorithm to prepare injective PEPS also provides a better scaling than the one presented in Ref. [7].

The class of states we consider in this Letter can be thought of as commuting finite range operators acting on a set of maximally entangled pair states (Fig. 1). More precisely, consider a regular lattice in some dimension, and let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be the associated (infinite) graph. We endow $\mathcal{G}$ with a distance d, the minimum number of edges separating two vertices in $\mathcal{V}$. We associate a d-dimensional Hilbert space, $\mathcal{H}_v$, to each of the vertices $v \in \mathcal{V}$. Consider the set $\mathbf{\Lambda}$ of interaction supports, i.e., $\mathbf{\Lambda}$ is a collection of sets of vertices whose relative distance is at most a constant R, the interaction length, and consider for each $\lambda \in \mathbf{\Lambda}$ an interaction Q_λ which is an operator supported on $\bigotimes_{v\in\lambda} \mathcal{H}_v$. We assume that they are strictly positive, $\mathbb{1} \geq Q_\lambda > q_0\mathbb{1}$, and mutually commute, $[Q_\lambda, Q_{\lambda'}] = 0$. Consider also a set $\mathbf{\Upsilon}$ of mutually excluding pairs of neighboring vertices. Moreover, let Λ_N be a finite subset of $\mathbf{\Lambda}$ with $|\Lambda_N| = N$, and define

$$|\phi_N\rangle \propto \prod_{\lambda\in\Lambda_N} Q_\lambda \bigotimes_{\mu\in\mathbf{\Upsilon}_N} |\phi^+\rangle_\mu, \tag{3}$$

where $\Upsilon_N = \{\mu \in \mathbf{\Upsilon} | \mu \cap (\bigcup_{\lambda\in\Lambda_N} \lambda) \neq \emptyset\}$ is the set of pairs with a vertex in Λ_N, and $|\phi^+\rangle = \sum_{i=1}^d |ii\rangle$ is an unnormalized maximally entangled state between the pairs of vertices in Υ_N. We will give a quantum algorithm to prepare the state, Eq. (3), and analyze the runtime as a function of N and other spectral properties. In the following, we drop the subindex N to ease the notation.

As mentioned above, Eq. (3) includes two relevant classes of states. The first is the class of injective PEPS. The graph is composed of nodes, each of them including a set of vertices [Fig. 2(a)]. In this case, Υ contains pairs of vertices in nearest neighbor nodes, whereas Λ contains each node. The operators Q_λ act on different nodes, and therefore trivially commute. The resulting state is just a PEPS, which is injective since each Q_λ is invertible. In fact, every injective PEPS can be expressed in this form up to a local unitary using a QR decomposition. The second class is the class of Gibbs states of commuting Hamiltonians [29]. To see this, consider the graph which contains sites composed of two vertices, one of them is called "system" and the other "ancilla." The set Υ contains all sites, whereas Λ contains interacting system vertices [Fig. 2(b)]. The relation with Gibbs states is evident if we write $Q_\lambda = e^{-\beta h_\lambda/2}$, where $\|h_\lambda\| < 1$, and take into account that they mutually commute. It is easy to see that if we trace the ancillas, we obtain

$$\rho \propto e^{-\beta H}, \tag{4}$$

where $H = \sum_{\lambda\in\Lambda} h_\lambda$.

The state Eq. (3) is the unique ground state of a frustration-free local Hamiltonian that can be written as

$$G = \sum_{\mu\in\Upsilon} G_\mu, \tag{5}$$

with

$$G_\mu = \left(\prod_{\lambda\in\Lambda_\mu} Q_\lambda^{-1}\right) P_\mu \left(\prod_{\lambda\in\Lambda_\mu} Q_\lambda^{-1}\right), \tag{6}$$

where $\Lambda_\mu = \{\lambda \in \Lambda | \lambda \cap \mu \neq \emptyset\}$ is the set of supports whose interactions act nontrivially on μ, and P_μ is the projector onto the subspace orthogonal to $|\phi^+\rangle_\mu$. Notice that since each G_μ is supported in a region of radius R around μ, G is indeed local.

The state Eq. (3) can be prepared using an adiabatic algorithm. For that, we define a path $Q_\lambda(s)$ with unique ground state $|\phi(s)\rangle$, where $s \in [0, 1]$, with $Q_\lambda(0) = \mathbb{1}$ and $Q_\lambda(1) = Q_\lambda$. We can choose $Q_\lambda(s) = (1-s)\mathbb{1} + sQ_\lambda$.

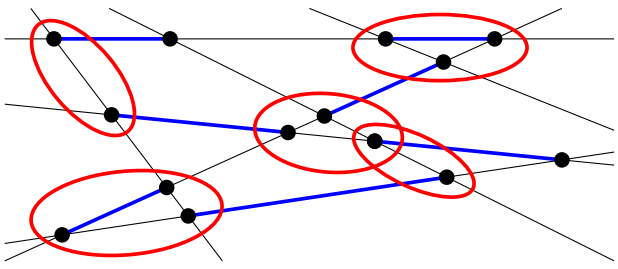

FIG. 1. The general class of states, Eq. (3). Finite range operators (red) acting on a collection of maximally entangled pair states (blue) distributed on a graph.

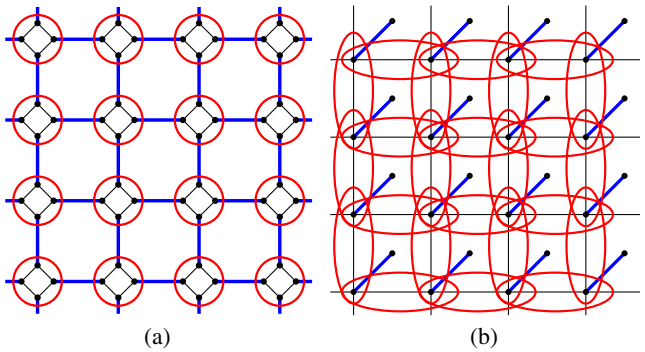

FIG. 2. (a) Projected entangled pair states. (b) Purification of a thermal state. For each system qudit, we introduce an ancilla to be placed in a maximally entangled pair with its system particle, then apply $e^{-\beta H/2}$ to the system.

In the case of the thermal state, we can also choose $Q_\lambda(s) = e^{-\beta s h_\lambda/2}$. Then, by starting with $|\phi(0)\rangle$ and changing the parameter $s: 0 \to 1$ sufficiently slowly, we will end up in the desired state $|\phi(1)\rangle$. The runtime for this preparation, as measured by the number of elementary quantum gates, is unpractical, however, as it scales as $T = O(N^4\Delta^{-3}\varepsilon^{-1}\mathrm{polylog}(N/\varepsilon))$, where ε is the tolerated error and Δ is the minimum spectral gap along the path. Indeed, the adiabatic theorem [30] gives an adiabatic runtime of $\tau = O(N^2\Delta^{-3}\varepsilon^{-1})$ so that Hamiltonian simulation [31] gives $T = O(\tau N^2\mathrm{polylog}(N/\varepsilon))$.

To obtain a better scaling, we first use a variant of the adiabatic theorem with almost exponentially better runtime dependence on the error using a sufficiently smooth reparameterization of the Hamiltonian path. The quadratic scaling of the runtime with the derivative of the Hamiltonian, however, leads to an unpractical dependence on N since the Hamiltonian contains $O(N)$ terms that change with time. To avoid this, we change the Q's individually, leading to an adiabatic runtime of $\tau = O(N\log^{1+\alpha}(N/\varepsilon\Delta)\Delta^{-3})$. This, however, uses Hamiltonians acting on the whole system, despite only the change of a single Q, which would result in an additional factor of $O(N^2\mathrm{polylog}(N/\varepsilon))$ for the computational time measured by the number of elementary gates. We circumvent this problem by using Lieb-Robinson bounds [32] and the frustration freeness to show that under the assumption of a uniformly lower bounded spectral gap, it is at each step sufficient to evolve with a Hamiltonian acting only on $O(\mathrm{polylog}(N/\varepsilon))$ sites instead of the full lattice.

Thus, define a sequence of N Hamiltonian paths by enumerating the elements of Λ as $\lambda_1, \ldots, \lambda_N$, and define

$$G_n(s) = \sum_{\substack{\mu\in\Upsilon \\ d(\mu,\lambda_n)<\chi\log^{1+\alpha}(N/\varepsilon)}} G_{n,\mu}(s) \tag{7}$$

for $n = 1, \ldots, N$, where χ is a constant control parameter, and

$$G_{n,\mu}(s) = \left(\prod_{\substack{m \\ \lambda_m\in\Lambda_\mu}} A^{-1}_{n,m}(s)\right) P_\mu \left(\prod_{\substack{m \\ \lambda_m\in\Lambda_\mu}} A^{-1}_{n,m}(s)\right) \tag{8}$$

with

$$A_{n,m}(s) = \begin{cases} Q_{\lambda_m}(1) & m < n \\ Q_{\lambda_m}(s) & m = n \\ Q_{\lambda_m}(0) = \mathbb{1} & m > n. \end{cases} \tag{9}$$

Notice that G_n is supported on a region of radius $O(\log^{1+\alpha}(N/\varepsilon))$ and dG_n/ds is supported on a region of bounded size. By reparameterizing $G_n(s) \to G_n(f(s))$ with f, a function in the Gevrey class $1+\alpha$, we can assume G_n to be in the same Gevrey class [33].

Consider the sequence of Schrödinger equations

$$i\frac{d}{dt}|\psi_n\rangle = G_n\left(\frac{t}{\tau_n}\right)|\psi_n\rangle, \qquad |\psi_{n+1}(0)\rangle = |\psi_n(\tau_n)\rangle \tag{10}$$

for times $\tau_n = O(\log(N/\varepsilon)^{1+\alpha})$, starting in $|\psi_1(0)\rangle = |\phi(0)\rangle$, the trivial ground state of $G_1(0)$. The algorithm proceeds by running Hamiltonian simulation [31] on this sequence of adiabatic evolutions. Since at all times we only evolve with Hamiltonians acting on $O(\mathrm{polylog}(N/\varepsilon))$ sites, the number of gates only grows as Eq. (1). Moreover, the evolution of consecutive G_n's can be parallelized if their support is disjoint, i.e., if $G_n, \ldots, G_{n+l}$ have disjoint supports, the subsequence can be replaced by their sum without altering the evolution. Since $|\mathrm{supp}G_n| = O(\mathrm{polylog}(N/\varepsilon))$, it is clear that an ordering of the λ_n can be chosen such that subsequences of length $\Omega(N/\mathrm{polylog}(N/\varepsilon))$ of the G_ns can be parallelized at a time, resulting in a circuit of depth Eq. (2), an almost exponential improvement over previous bounds.

In the following, we show that for a uniformly lower bounded gap, the error of the above algorithm is bounded by ε. First, we use that under sufficient smoothness conditions on a Hamiltonian path $G(s)$, the final error can be almost exponentially small in the adiabatic runtime. Indeed, as proven in the Supplemental Material [36], if G is in the Gevrey class $1+\alpha$ and $d^kG/ds^k = 0$ at $s = 0, 1$ for all $k \geq 1$, then an adiabatic runtime of

$$\tau = O\left(\log^{1+\alpha}\left(\frac{K}{\varepsilon\Delta}\right)\frac{K^2}{\Delta^3}\right) \tag{11}$$

is sufficient for an error ε, where Δ is the minimum gap of $G(s)$ and $K = |\mathrm{supp}dG/ds|$ if G is local. The required smoothness conditions can always be achieved with a suitable reparametrization of the path $G(s) \to G(f(s))$.

This allows us to implement the global change of the Hamiltonian, Eq. (5), as a sequence of N local changes. Define the sequence of Hamiltonian paths,

$$\tilde{G}_n(s) = \sum_{\mu\in\Upsilon} G_{n,\mu}(s). \tag{12}$$

Notice that Eq. (12) is the same as Eq. (7), but contains all local terms $G_{n,\mu}$. The weak dependence on ε^{-1} in Eq. (11) ensures that the accumulated error under the sequential evolution with Eq. (12) remains small. Indeed, for a final error ε, it is sufficient that the evolution with each $\tilde{G}_n$ in this sequence only generates an error of at most ε/N. Equation (11) and $|\mathrm{supp}d\tilde{G}_n/ds| = O(1)$ imply that this can be achieved in a time $\tau_n = O(\log^{1+\alpha}(N/\varepsilon\Delta_n)\Delta_n^{-3})$, where Δ_n is the minimum spectral gap of $\tilde{G}_n$. A decomposition into a circuit then requires $T = O(N^3\mathrm{polylog}(N/\varepsilon\Delta)\Delta^{-3})$ elementary gates, where $\Delta = \min_n\Delta_n$. This is already an improvement by a factor N over the naive change of the entire Hamiltonian, assuming similar behaviour of Δ compared to the spectral gap of the original path $G(s)$.

Assuming that $\Delta = \Omega(1)$, we can further improve on this using Lieb-Robinson bounds to localize the effect of the adiabatic change. Indeed, we show in the Supplemental Material [36] that local terms in Eq. (12) which are supported at a distance $\Omega(\log^{1+\alpha}(N/\varepsilon))$ away from the support of $d\tilde{G}_n/ds$ do not significantly contribute to the unitary evolution generated by Eq. (12). This allows the replacement of Eq. (12) with Eq. (7) without significantly altering the evolution and thus the final state. Notice that G_n only acts on $O(\text{polylog}(N/\varepsilon))$ sites and $\tau_n = O(\text{polylog}(N/\varepsilon))$ for all n. Thus, its unitary evolution can be simulated with only $O(\text{polylog}(N/\varepsilon))$ gates. Hence, we finally obtain a number of gates in the circuit model that grows only as Eq. (1) for a constant error and lower bounded spectral gap. Using the described parallelization, we finally obtain a circuit depth, Eq. (2), as claimed.

In the analysis above, we have assumed a gap $\geq \Delta$ along all N paths. This assumption can in fact be relaxed to a gap at either $s = 0$ or $s = 1$ (see Supplemental Material [36]), using the positivity condition on Q_λ. We thus say that the system has a uniformly lower bounded gap Δ if for all finite subsets $\Lambda \subset \mathbf{\Lambda}$, the Hamiltonian, Eq. (5), has a spectral gap $\geq \Delta$. Under this assumption [47], the circuit depth, Eq. (2), can be guaranteed [48].

For the preparation of thermal states of classical Hamiltonians H, it is natural to compare these results with the performance of classical Monte Carlo Markov chain algorithms for Gibbs sampling such as the Metropolis algorithm or Glauber dynamics. Notice that due to the nature of their implementation, a fair comparison of performance should compare the mixing time of a discrete-time Markov chain to the number of elementary quantum gates, whereas the mixing time of a continuous-time Markov chain should be compared to the circuit depth. The best known upper bound on the discrete mixing time for Monte Carlo Markov chain algorithms for sampling from Gibbs distributions of classical Hamiltonians given just the promise of a spectral gap scales as $O(N^2)$. Although under certain additional assumptions such as translational invariance [49,50], weak mixing in two dimensions [51], or high temperature [52], the existence of a logarithmic Sobolev constant and hence the rapid (discrete) mixing time of $O(N \log N)$ can be proven, no such proof exists for the general case to the best of our knowledge. Our scheme thus outperforms classical Monte Carlo algorithms whenever rapid mixing cannot be shown even in the presence of a uniform gap.

Note that any classical Monte Carlo algorithm can be realized as an adiabatic algorithm, as has, e.g., been observed in Ref. [20]. Indeed, if S is the generator matrix of a continuous-time Monte Carlo algorithm that satisfies detailed balance with respect to the Gibbs distribution, $G = -e^{\beta H/2} S e^{-\beta H/2}$ is Hermitian. This Hamiltonian has the same spectrum as $-S$ and has the unique ground state $e^{-\beta H/2}|+\rangle^{\otimes N}$. For classical Hamiltonians H, this state has the same measurement statistics as ρ_β for observables that are products of σ_Z. By introducing an ancilla for every particle and applying the map $|i\rangle \mapsto |ii\rangle$, the purified version of the thermal state can also be recovered, and its parent Hamiltonian has the same spectrum as $-S$ within the symmetric subspace. Thus, any classical system with a uniform spectral gap for the generator matrix can be turned into a rapid adiabatic algorithm.

For quantum Hamiltonians, notice the restriction to commuting local terms. For noncommuting local terms, an approximate quasilocal parent Hamiltonian can be considered above some constant temperature that allows the preparation in polynomial time. We describe this procedure in the Supplemental Material [36].

For the preparation of injective PEPS, the given algorithm is similar to Ref. [7], which, however, requires a runtime of $O(N^4)$ in the uniformly gapped case, due to the use of phase estimation and the "Marriot-Watrous trick," which are computationally expensive for large systems. The better runtime of the present algorithm is largely due to replacing these subroutines by a local adiabatic change.

Throughout the analysis of this Letter, we focused on the case where a uniform constantly lower-bounded spectral gap is assumed. This assumption is only used to obtain a small number of elementary gates and circuit depth, whereas the adiabatic runtime of $\tau = O(N \log^{1+\alpha}(N/\varepsilon\Delta)\Delta^{-3})$ is independent of this assumption [53]. In contrast, the runtime of the algorithm to prepare PEPS given in Ref. [7] only grows as $T \sim \Delta^{-1}$ for small gaps, and for thermal states, algorithms based on quantum walks, phase estimation, and the quantum Zeno effect have been proposed with a runtime of $T \sim \Delta^{-1/2}$ [12,21,22], albeit with worse scaling in the system size. We believe that similar techniques can be applied to our scheme of local changes to obtain a good scaling of the runtime for both large system sizes and small spectral gaps. Moreover, it would be interesting to investigate if this scheme of local changes can also be applied to speed up *classical* Monte Carlo algorithms.

We have also shown that the algorithm can be parallelized, thus giving rise to a circuit depth that scales only polylogarithmically with N. This is particularly attractive for certain experimental realizations of analog quantum simulators, such as with atoms in optical lattices [54] or trapped ions [55], where this could be carried out in a very natural way.

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Rapid adiabatic preparation of injective PEPS and Gibbs sates: Supplemental Material

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I. PROOF OF THE ADIABATIC THEOREM WITH ALMOST EXPONENTIAL ERROR DECAY

In this section, we prove a variant of the adiabatic theorem that only requires a runtime almost exponentially small in the allowed error. Our proof largely follows the proof given in [1], which is based on the method of adiabatic expansion [2]. The adiabatic expansion in [2] establishes an approximation of the time-dependent Schrödinger evolution in terms of the instantaneous ground state and its derivatives, but on its own does not necessarily imply an adiabatic theorem because it assumes a special initial state. Our proof, like [1], resolves this problem by exploiting the Gevrey-class condition which allows to satisfy these initial conditions, and uses this expansion to establish a bound on the required runtime. However, unlike [1], which only proves the almost exponential dependence of the runtime with respect to accuracy, our proof also explicitly establishes the dependence on all other parameters such as the spectral gap and the bound on the Hamiltonian derivatives [3].

Consider a smooth path of Hamiltonians, $G(s)$, $s \in [0,1]$, acting on a finite-dimensional Hilbert space $\mathcal{H}$. Let $\phi(s)$ [4] be the ground state of $G(s)$ and $\psi(\epsilon, s)$ the solution of the following Schrödinger equation:

$$i\epsilon\dot{\psi}(\epsilon,s) = G(s)\psi(\epsilon,s), \quad \psi(0) = \phi(0), \tag{13}$$

where $1/\epsilon = \tau$ is the runtime of the adiabatic algorithm, and $\dot{}$ denotes derivative with respect to s. We assume furthermore that the ground state energy of $G(s)$ is 0 (i.e., we fix the phase of ψ) and that it has a gap at least Δ throughout the whole path. By an appropriate choice of the phase of ϕ, we can without loss of generality assume that $\left\langle \dot{\phi}(s) \middle| \phi(s) \right\rangle = 0$. In the following, we will sometimes drop the explicit dependence on s to simplify the notation. Unless otherwise stated, $\|.\|$ will always denote the operator norm for operators and the Euclidean vector norm for vectors (it will always be clear from the context which one is used). In this section, we prove the following theorem.

Theorem 1. *Suppose that all derivatives of G vanish at 0 and at 1, and moreover that it satisfies the following Gevrey condition: there exist non-negative constants K, c and α such that for all $k \geq 1$,*

$$\|G^{(k)}\| \leq K c^k \frac{[k!]^{1+\alpha}}{(k+1)^2}. \tag{14}$$

Then,

$$\min_\theta \|\psi(\epsilon,1) - e^{i\theta}\phi(1)\| \leq 8ce\frac{K}{\Delta}\left(\frac{4\pi^2}{3}\right)^3 \cdot \exp\left\{-\left(\frac{1}{4ec^2}\left(\frac{3}{4\pi^2}\right)^5 \tau\frac{\Delta^3}{K^2}\right)^{\frac{1}{1+\alpha}}\right\}. \tag{15}$$

Notice that we don't require the Gevrey condition (14) to hold for $k = 0$. Therefore, in the application of Theorem 1 in the main text, $K = O(1)$ since along the paths $\tilde{G}_n(s)$ (as defined in (12) in the main text), only $O(1)$ local terms change.

Proof of Theorem 1. Following the adiabatic expansion method from [1, 2], we search $\psi(\epsilon, s)$ in the form of an asymptotic series expansion by constructing vectors $\phi_j(s)$, $s \in [0,1]$, $j \geq 0$, such that for all $M > 0$,

$$\left\| \psi(\epsilon,s) - \sum_{j=0}^{M-1} \phi_j(s)\epsilon^j \right\| = O(\epsilon^M). \tag{16}$$

We first show an explicit expression for ϕ_j provided that such an expansion exists. Second,we prove that the expansion really exists if $G^{(k)}(0) = 0$ for all k by giving an explicit error bound. Third, to connect the expansion to the adiabatic theorem, we show that

$$\min_\theta \|\psi(\epsilon,1) - e^{i\theta}\phi(1)\| \leq 2\|\psi(\epsilon,1) - \sum_{j=0}^{M-1}\phi_j(s)\epsilon^j\|, \tag{17}$$

for some θ for all M if $G^{(k)}(1) = 0$ for all k. This already proves an error bound of $O(\epsilon^M)$ for any M. Finally, if G is Gevrey class, then the error bound can be expressed with the help of the parameters appearing in the Gevrey condition and using a suitable choice of M yields to the bound in Eq. (15).

Explicit form of ϕ_j. To satisfy the equation at $s = 0$, we require $\phi_0(0) = \phi(0)$ and $\phi_j(0) = 0$ for all $j > 0$. Furthermore, substituting back the ansatz to the Schrödinger equation Eq.(13), following [2], we arrive at the recursion

$$\phi_j = \varphi_j \phi + iG^{-1}\dot{\phi}_{j-1}, \quad \varphi_j = i\int_0^t \mathrm{d}t' \left\langle \dot{\phi}(t') \right| G^{-1}(t') \left| \dot{\phi}_{j-1}(t') \right\rangle, \tag{18}$$

for all $j > 0$, where $\varphi_j(s)$ is a complex number and G^{-1} is the pseudo-inverse of G, and initial values are

$$\phi_0(s) = \phi(s) \tag{19}$$
$$\varphi_0(s) = 1. \tag{20}$$

Note that $\varphi_j(0)$ has to be zero in order for $\phi_j(0)$ to be zero, but this is not a sufficient condition. We will investigate below when $\phi_j(0) = 0$ can be satisfied.

Existence of the expansion. To satisfy $\phi_j(0) = 0$ for $j > 0$, $\dot{\phi}_{j-1}(0)$ needs to be parallel to $\phi(0)$. This is satisfied if all derivatives of G are 0 at $s = 0$ (see Lemma 2 below). We show that if this condition is fulfilled, then the expansion exists.

Define the truncation of the asymptotic series expansion,

$$\psi_M = \sum_{j=0}^{M-1} \phi_j \epsilon^j. \tag{21}$$

Note that if $\|\psi - \psi_M\| = O(\epsilon^{M-1})$, then the expansion exists. Indeed, then $\|\psi - \psi_M\| = \|\psi - \psi_{M+1} + \epsilon^M \phi_M\| = O(\epsilon^M)$. By construction, ψ_M almost satisfies the Schrödinger equation: $i\epsilon\dot{\psi}_M = G\psi_M + i\epsilon^M \dot{\phi}_{M-1}$. Let $U(s)$ be the dynamics generated by G/ϵ. Then, $\|\psi_M(\epsilon, s) - \psi(\epsilon, s)\| = \|U(s)^\dagger \psi_M(\epsilon, s) - \phi(0)\|$ and

$$\left\|U(s)^\dagger \psi_M(\epsilon, s) - \phi(0)\right\| = \left\|\int_0^s \mathrm{d}s' \frac{\mathrm{d}}{\mathrm{d}s'} \left(U^\dagger \psi_M\right)\right\| = \left\|\epsilon^{M-1} \int_0^s \mathrm{d}s' U^\dagger \dot{\phi}_{M-1}\right\| \leq \epsilon^{M-1} \int_0^s \mathrm{d}s' \left\|\dot{\phi}_{M-1}\right\|, \tag{22}$$

where we used that if the first M derivatives of G are 0, then $\psi_M(\epsilon, 0) = \phi(0)$. This proves the existence of the expansion.

Connecting the expansion to the adiabatic theorem. Using the triangle inequality, we obtain

$$\min_\theta \|\psi(\epsilon, 1) - e^{i\theta}\phi(1)\| \leq \|\psi(\epsilon, 1) - \psi_M(\epsilon, 1)\| + \min_\theta \|\psi_M(\epsilon, 1) - e^{i\theta}\phi(1)\|. \tag{23}$$

In Lemma 2, we prove that if the first M derivatives of $G(s)$ vanish at $s = 1$, then $\phi_j(1)$ is parallel to $\phi(1)$ for all $j = 1, \ldots, M$. Therefore, $\psi_M(\epsilon, 1)$ is parallel to $\phi(1)$, so that $\min_\theta \|\psi_M(\epsilon, 1) - e^{i\theta}\phi(1)\| = |\|\psi_M(\epsilon, 1)\| - 1|$. But $1 = \|\psi(\epsilon, 1)\|$, so using the triangle inequality, we get $\min_\theta \|\psi_M(\epsilon, 1) - e^{i\theta}\phi(1)\| \leq \|\psi_M(\epsilon, 1) - \psi(\epsilon, 1)\|$. Therefore,

$$\min_\theta \|\psi(\epsilon, 1) - e^{i\theta}\phi(1)\| \leq 2\|\psi(\epsilon, 1) - \psi_M(\epsilon, 1)\|. \tag{24}$$

Choice of M. From Eq. (22) and (24),

$$\min_\theta \|\psi(\epsilon, 1) - e^{i\theta}\phi(1)\| \leq 2\|\psi(\epsilon, 1) - \psi_M(\epsilon, 1)\| \leq 2\epsilon^{M-1} \int_0^1 \|\dot{\phi}_{M-1}\|, \tag{25}$$

so we only need to bound $\|\dot{\phi}_{M-1}\|$. We do this by using that G is Gevrey class. From Lemma 7 below,

$$\|\dot{\phi}_{M-1}\| \leq 2\frac{4\pi^2}{3} \cdot 2c\frac{K}{\Delta}\left(\frac{4\pi^2}{3}\right)^2 \cdot \left[\frac{K^2}{\Delta^3} 4c^2 \left(\frac{4\pi^2}{3}\right)^5\right]^{M-1} \frac{[M!]^{1+\alpha}}{(M+1)^2}. \tag{26}$$

Therefore,

$$\|\psi(\epsilon, 1) - \phi(1)\| \leq \epsilon^{M-1} \cdot 8c\frac{K}{\Delta}\left(\frac{4\pi^2}{3}\right)^3 \cdot \left[\frac{K^2}{\Delta^3} 4c^2 \left(\frac{4\pi^2}{3}\right)^5\right]^{M-1} \frac{[M!]^{1+\alpha}}{(M+1)^2}. \tag{27}$$

Changing M to $M+1$ and using that $[(M+1)!]^{1+\alpha}/(M+2)^2 \leq M^{(1+\alpha)M}$, we obtain

$$\|\psi(\epsilon,1)-\phi(1)\| \leq 8c\frac{K}{\Delta}\left(\frac{4\pi^2}{3}\right)^3 \cdot \left[\frac{K^2}{\Delta^3}4c^2\left(\frac{4\pi^2}{3}\right)^5 \frac{M^{1+\alpha}}{\tau}\right]^M. \tag{28}$$

This is true for any M, so setting

$$M = \left\lfloor \left(\frac{\tau\Delta^3}{eK^2 4c^2\left(\frac{4\pi^2}{3}\right)^5}\right)^{\frac{1}{1+\alpha}} \right\rfloor, \tag{29}$$

we obtain

$$\|\psi(\epsilon,1)-\phi(1)\| \leq 8ce\frac{K}{\Delta}\left(\frac{4\pi^2}{3}\right)^3 \cdot \exp\left\{-\left(\tau\frac{\Delta^3}{K^2}\frac{1}{4ec^2}\left(\frac{3}{4\pi^2}\right)^5\right)^{\frac{1}{1+\alpha}}\right\}. \tag{30}$$

This proves Theorem 1. □

We have repeatedly used the following lemma in the proof of Theorem 1.

Lemma 2. *If $G^{(k)}(s_0)=0$ for some $s_0 \in [0,1]$ and for all $k=1\dots M$, then*

(i) $\phi^{(k)}(s_0)$ is parallel to $\phi(s_0)$ for all $k=0,\dots,M$,

(ii) $\left[G^{(-1)}\right]^{(k)}(s_0)=0$ for all $k=1,\dots,M$,

(iii) $\phi_k^{(l)}(s_0)$ is parallel to $\phi(s_0)$ for all $k=0,\dots,M$ and $l=0,\dots,M-k$.

Proof. $G\phi=0$, so $(G\phi)^{(k)}=\sum_{j=0}^k \binom{k}{j} G^{(j)}\phi^{(k-j)}=0$ for all k. Applying this for $k\leq M$ and evaluating the result at s_0, the derivatives of G vanish, thus $G\phi^{(k)}=0$ and therefore $\phi^{(k)}$ is parallel to ϕ at s_0, which proves (i).

To prove (ii), use the Cauchy formula

$$G^{-1} = \frac{1}{2\pi}\oint_\Gamma (z-G)^{-1}\frac{1}{z}\mathrm{d}z, \tag{31}$$

where $\Gamma=\{z\in\mathbb{C}\mid |z|=\Delta/2\}$ is a fixed curve around 0. Taking the kth derivative of Eq. (31) and evaluating it at s_0, we see that the derivatives of G^{-1} also disappear.

To prove (iii), we proceed by induction on k. By (i), the claim is true for $k=0$. For $k>0$, we have $\phi_k^{(l)} = (\varphi_k\phi)^{(l)} + i(G^{-1}\phi_{k-1}^{(1)})^{(l)}$. By (i), the first term is parallel to ϕ at s_0. The second term consists of derivatives of G^{-1} and derivatives of $\phi_k^{(1)}$. By (ii), the derivatives of G^{-1} vanish at s_0, so that the only remaining term is $iG^{-1}\phi_{k-1}^{(l+1)}$. But this term also vanishes at s_0 by the induction hypothesis. This proves (iii). □

In the remainder of this section, we derive the bound on the norm of $\dot\phi_{M-1}$ which was used in the proof of Theorem 1, following the analysis in [1]. First, we recall two technical lemmas from [1], which will be used repeatedly.

Lemma 3. *Let p,q be non-negative integers and $r=p+q$. Then,*

$$\sum_{l=0}^k \binom{k}{l}\frac{[(l+p)!(k-l+q)!]^{1+\alpha}}{(l+p+1)^2(k-l+q+1)^2} \leq \frac{[(k+r)!]^{1+\alpha}}{(k+r+1)^2}\frac{4\pi^2}{3}. \tag{32}$$

Proof. Notice that if $r=p+q$, then

$$\binom{k}{l}[(l+p)!(k+q-l)!]^{1+\alpha} = \frac{\binom{k}{l}[(k+r)!]^{1+\alpha}}{\binom{k+r}{l+p}^{1+\alpha}} \leq [(k+r)!]^{1+\alpha}. \tag{33}$$

To upper-bound the summation, divide the sum into two parts at $\lfloor (k-p+q)/2\rfloor$. If $l<\lfloor (k-p+q)/2\rfloor$, then $(k-l+q+1) > \lfloor (k+p+q)/2\rfloor+1$. Otherwise, if $l\geq\lfloor (k-p+q)/2\rfloor$, then $(l+p+1)\geq\lfloor (k+p+q)/2\rfloor+1$. Therefore,

$$\sum_{l=0}^k \frac{1}{(l+p+1)^2(k-l+q+1)^2} \leq 2\sum_{l=0}^\infty \frac{1}{(l+1)^2}\frac{1}{(\lfloor (k+p+q)/2\rfloor+1)^2}. \tag{34}$$

This can be upper-bounded by $4\pi^2/3$ as $k+p+q+1\leq 2(\lfloor (k+p+q)/2\rfloor+1)$. This finishes the proof of Lemma 3. □

We now use Lemma 3 to prove that if A and B are Gevrey-class, then their product is also Gevrey-class.

Lemma 4. *Let $A(s), B(s)$ ($s \in [0,1]$) be smooth paths of either vectors in $\mathcal{H}$ or operators in $\mathcal{B}(\mathcal{H})$ satisfying*

$$\|A^{(k)}\| \leq C d^k \frac{[(k+p)!]^{1+\alpha}}{(k+p+1)^2} \quad \text{and} \quad \|B^{(k)}\| \leq E f^k \frac{[(k+q)!]^{1+\alpha}}{(k+q+1)^2} \tag{35}$$

for some non-negative constants C, d, E, f, non-negative integers p, q, and for all $k \geq 0$. Then,

$$\|(AB)^{(k)}\| \leq \frac{4\pi^2}{3} C E g^k \frac{[(k+r)!]^{1+\alpha}}{(k+r+1)^2} \tag{36}$$

for all $k \geq 0$, where $g = max(d, f)$ and $r = p + q$.

Proof. We have

$$\|(AB)^{(k)}\| \leq \sum_l \binom{k}{l} \|A^{(l)}\| \|B^{(k-l)}\|, \tag{37}$$

so inserting the bounds (35) and upper-bounding d and f by g, we obtain

$$\|(AB)^{(k)}\| \leq C E g^k \sum_l \binom{k}{l} \frac{[(l+p)!]^{1+\alpha}}{(l+p+1)^2} \frac{[(k-l+q)!]^{1+\alpha}}{(k-l+q+1)^2}. \tag{38}$$

Using Lemma 3 to upper-bound the r.h.s. of this expression proves Lemma 4. □

Next we give a bound on the derivatives of the pseudo-inverse G^{-1}. As G is non-invertible, the proof consists of two steps: first reducing the problem to the invertible case, then proving that the inverse of an invertible Gevrey-class operator is again Gevrey-class (assuming that the inverse is uniformly bounded).

Lemma 5. *If G satisfies Eq. (14), then for all $k \geq 0$,*

$$\|(G^{-1})^{(k)}\| \leq \frac{2}{\Delta} \left(\frac{K}{\Delta} 2c \frac{4\pi^2}{3} \right)^k \frac{[k!]^{1+\alpha}}{(k+1)^2}. \tag{39}$$

Proof. First, write the pseudo-inverse using the Cauchy formula,

$$G^{-1} = \frac{1}{2\pi i} \oint_\Gamma \frac{1}{G - z} \frac{1}{z} \mathrm{d}z, \tag{40}$$

where $\Gamma = \{z \in \mathbb{C} \big| |z| = \Delta/2\}$ is a fixed, s-independent curve. Taking the kth derivative of Eq. (40) (with respect to s), we get

$$(G^{-1})^{(k)} = \frac{1}{2\pi i} \oint_\Gamma [(G - z)^{-1}]^{(k)} \frac{1}{z} \mathrm{d}z. \tag{41}$$

Thus, the norm of the pseudo-inverse can be bounded by the triangle inequality,

$$\|(G^{-1})^{(k)}\| \leq \max_{z \in \Gamma} \|[(G - z)^{-1}]^{(k)}\|. \tag{42}$$

Note that $G - z$ is invertible and $\|(G - z)^{-1}\| \leq 2/\Delta$ for $z \in \Gamma$. We now show that $(G - z)^{-1}$ is also Gevrey-class, more precisely that

$$\left\| \left[(G - z)^{-1}\right]^{(k)} \right\| \leq \frac{2}{\Delta} \left(\frac{2}{\Delta} K c \frac{4\pi^2}{3} \right)^k \frac{[k!]^{1+\alpha}}{(k+1)^2} \tag{43}$$

for $k \geq 0$. To show this, we proceed by induction. For $k = 0$, the bound obviously holds. Taking the kth derivative of $(G - z)(G - z)^{-1} = \mathbb{1}$, we get

$$\left[(G - z)^{-1}\right]^{(k)} = (G - z)^{-1} \sum_{l=1}^{k} \binom{k}{l} (G - z)^{(l)} \left[(G - z)^{-1}\right]^{(k-l)}. \tag{44}$$

Using the induction hypothesis and collecting terms (notice that $l \geq 1$ and $k - l \leq k - 1$), we get

$$\left\| \left[(G - z)^{-1} \right]^{(k)} \right\| \leq \frac{2}{\Delta} \left(\frac{2}{\Delta} Kc \right)^k \left(\frac{4\pi^2}{3} \right)^{k-1} \sum_{l=1}^{k} \binom{k}{l} \frac{[l!(k-l)!]^{1+\alpha}}{(l+1)^2 (k-l+1)^2}. \tag{45}$$

Using Lemma 3 to upper-bound the sum in (45), we get

$$\left\| \left[(G - z)^{-1} \right]^{(k)} \right\| \leq \frac{2}{\Delta} \left(\frac{2}{\Delta} Kc \frac{4\pi^2}{3} \right)^k \frac{[k!]^{1+\alpha}}{(k+1)^2}. \tag{46}$$

This proves (43). Substituting this bound into Eq. (42) proves Lemma 5. □

Next, we prove that the ground state is also Gevrey-class (with the special choice of the phase as above).

Lemma 6. *If G satisfies Eq. (14), then the ground state ϕ satisfies*

$$\left\| \phi^{(k)} \right\| \leq \left(2c \frac{K}{\Delta} \left(\frac{4\pi^2}{3} \right)^2 \right)^k \frac{[k!]^{1+\alpha}}{(k+1)^2}. \tag{47}$$

for all $k \geq 0$, where K, c and α are defined in Eq. (14) and Δ is the minimal gap of G.

Proof. We proceed by induction on k. For $k = 0$, (47) just reads $\|\phi\| \leq 1$. For $k > 0$, notice that $G\phi = 0$ and $\phi^{(1)} = -G^{-1} G^{(1)} \phi$ since the phase of ϕ is chosen such that $\left\langle \dot{\phi} \middle| \phi \right\rangle = 0$. Therefore,

$$\left\| \phi^{(k)} \right\| = \left\| \left[G^{-1} G^{(1)} \phi \right]^{(k-1)} \right\|. \tag{48}$$

Expanding the derivatives, we get

$$\left\| \phi^{(k)} \right\| \leq \sum_{l=0}^{k-1} \binom{k-1}{l} \left\| \left[G^{-1} G^{(1)} \right]^{(k-l-1)} \right\| \left\| \phi^{(l)} \right\|. \tag{49}$$

The right hand side can be bounded using the induction hypothesis as the higest derivative of ϕ appearing there is the $(k-1)$th. For that, we first derive a bound on the norm of the derivatives of $G^{-1} G^{(1)}$. This can be done by applying Lemma 4 to $G^{(1)}$ and G^{-1} and using Lemma 5 to obtain

$$\left\| [G^{-1} G^{(1)}]^{(k)} \right\| \leq \left(Kc \frac{2}{\Delta} \frac{4\pi^2}{3} \right)^{k+1} \frac{[(k+1)!]^{1+\alpha}}{(k+2)^2} \tag{50}$$

for $k \geq 0$. Substituting this bound into (49), we obtain

$$\|\phi^{(k)}\| \leq \sum_{l=0}^{k-1} \binom{k-1}{l} \left(Kc \frac{2}{\Delta} \frac{4\pi^2}{3} \right)^{k-l} \frac{[(k-l)!]^{1+\alpha}}{(k-l+1)^2} \left(Kc \frac{2}{\Delta} \left(\frac{4\pi^2}{3} \right)^2 \right)^l \frac{[l!]^{1+\alpha}}{(l+1)^2}. \tag{51}$$

Notice that $l \leq k - 1$, so

$$\|\phi^{(k)}\| \leq \left(Kc \frac{2}{\Delta} \frac{4\pi^2}{3} \right)^k \left(\frac{4\pi^2}{3} \right)^{k-1} \sum_{l=0}^{k-1} \binom{k-1}{l} \frac{[(k-l)!]^{1+\alpha}}{(k-l+1)^2} \frac{[l!]^{1+\alpha}}{(l+1)^2}. \tag{52}$$

Thus, using Lemma 3, we obtain

$$\left\| \phi^{(k)} \right\| \leq \left(Kc \frac{2}{\Delta} \left(\frac{4\pi^2}{3} \right)^2 \right)^k \frac{[k!]^{1+\alpha}}{(k+1)^2}, \tag{53}$$

which proves Lemma 6. □

We are now in the position to bound $\|\dot{\phi}_{M-1}\|$. Instead of bounding it directly, we prove a general bound on all $\|\phi_j^{(k)}\|$. The desired bound is obtained then by setting $j = M-1$ and $k = 1$.

Lemma 7. *For all $j, k \geq 0$, the vectors ϕ_j and scalars φ_j defined in Eq. (18) satisfy*

$$\|\phi_j^{(k)}\| \leq A_1 A_2^j A_3^k \frac{[(k+j)!]^{1+\alpha}}{(k+j+1)^2} \quad \text{and} \quad |\varphi_j^{(k)}| \leq A_2^j A_3^k \frac{[(k+j)!]^{1+\alpha}}{(k+j+1)^2}, \tag{54}$$

where the constants A_1, A_2 and A_3 can be expressed with the constants appearing in Eq. (14):

$$A_1 = \frac{8\pi^2}{3}, \quad A_3 = 2c\frac{K}{\Delta}\left(\frac{4\pi^2}{3}\right)^2, \quad A_2 = 4c^2\frac{K^2}{\Delta^3}\left(\frac{4\pi^2}{3}\right)^5. \tag{55}$$

Proof. We proceed by induction on j, using the recursion in relation (18). We first bound $|\varphi_j|$ using the induction hypothesis, then bound $|\varphi_j^{(k)}|$ for $k > 0$ before bounding $\|\phi_j^{(k)}\|$.

Base case. We have $\varphi_0(s) = 1$ and $\phi_0(s) = \phi(s)$, so (54) holds for $j = 0$ since

$$A_1 \geq 1 \quad \text{and} \quad A_3 \geq 2c\frac{K}{\Delta}\left(\frac{4\pi^2}{3}\right)^2. \tag{56}$$

Bound on $|\varphi_j|$, $j \geq 1$. $|\varphi_j|$ can be bounded by the maximum value of the integrand in Eq. (18),

$$|\varphi_j| \leq \|G^{-1}\dot{\phi}\|\|\dot{\phi}_{j-1}\| \leq \|G^{-1}\| \cdot \|\dot{\phi}\| \cdot \|\dot{\phi}_{j-1}\|. \tag{57}$$

Using the bound on $\|\dot{\phi}\|$ from Lemma 6, $\|G^{-1}\|$ from Lemma 7 and the induction hypothesis on $\|\dot{\phi}_{j-1}\|$, we get

$$|\varphi_j| \leq \frac{2}{\Delta} \cdot A_3 \frac{1}{4} \cdot A_1 A_2^{j-1} A_3 \frac{[(j)!]^{1+\alpha}}{(j+1)^2} \leq A_2^j \frac{[(j)!]^{1+\alpha}}{(j+1)^2} \tag{58}$$

since

$$1 \geq A_1 \frac{A_3^2}{A_2} \frac{2}{\Delta} \frac{1}{4}. \tag{59}$$

Bound on $\|\varphi_j^{(k)}\|$. We now bound $|\varphi_j^{(k)}|$ for $k > 0$. First, from the induction hypothesis,

$$\|\dot{\phi}_{j-1}^{(k)}\| \leq A_1 A_2^{j-1} A_3^{k+1} \frac{[(k+j)!]^{1+\alpha}}{(k+j+1)^2}. \tag{60}$$

Then, using Lemma 4 and Lemma 5, we get that for all $k \geq 0$,

$$\left\| \left(G^{-1}\dot{\phi}_{j-1}\right)^{(k)} \right\| \leq \frac{4\pi^2}{3} \frac{2}{\Delta} A_1 A_2^{j-1} A_3^{k+1} \frac{[(k+j)!]^{1+\alpha}}{(k+j+1)^2}. \tag{61}$$

Moreover, from Lemma 6,

$$\|\dot{\phi}^{(k)}\| \leq A_3^{k+1} \frac{[(k+1)!]^{1+\alpha}}{(k+2)^2}. \tag{62}$$

Since $\dot{\varphi}_j = \left\langle \dot{\phi} \middle| G^{-1}\dot{\phi}_{j-1} \right\rangle$, Lemma 4, Eq. (61) and (62) imply that

$$|\varphi_j^{(k+1)}| = |\dot{\varphi}_j^{(k)}| \leq \left(\frac{4\pi^2}{3}\right)^2 \frac{2}{\Delta} A_3 A_1 A_2^{j-1} A_3^{k+1} \frac{[(k+j+1)!]^{1+\alpha}}{(k+j+2)^2} \tag{63}$$

for $k \geq 0$. Changing $k+1$ to k gives

$$|\varphi_j^{(k)}| \leq \left(\frac{4\pi^2}{3}\right)^2 \frac{2}{\Delta} A_3 A_1 A_2^{j-1} A_3^k \frac{[(k+j)!]^{1+\alpha}}{(k+j+1)^2} \leq A_2^j A_3^k \frac{[(k+j)!]^{1+\alpha}}{(k+j+1)^2}, \tag{64}$$

since $1 \geq A_1 \frac{A_3}{A_2} \frac{2}{\Delta} \left(\frac{4\pi^2}{3}\right)^2$.

Bound on $\|\phi_j^{(k)}\|$. We now bound $\|\phi_j^{(k)}\|$. Using the bound on $\|\phi^{(k)}\|$ from Lemma 6 and $|\varphi_j^{(k)}|$, Lemma 4 implies

$$\|(\varphi_j\phi)^k\| \leq \frac{4\pi^2}{3} A_2^j A_3^k \frac{[(k+j)!]^{1+\alpha}}{(k+j+1)^2}. \tag{65}$$

Finally, using Eq. (18),

$$\|\phi_j^{(k)}\| \leq 2\max\left(\left\| (\varphi_j\phi)^{(k)} \right\|, \left\| \left(G^{-1}\dot{\phi}_{j-1} \right)^{(k)} \right\| \right). \tag{66}$$

Hence, since

$$2\frac{4\pi^2}{3} \leq A_1 \quad \text{and} \quad \frac{4\pi^2}{3}\frac{2}{\Delta} A_3 \leq A_2, \tag{67}$$

we obtain

$$\|\phi_j^{(k)}\| \leq A_1 A_2^j A_3^k \frac{[(k+j)!]^{1+\alpha}}{(k+j+1)^2}, \tag{68}$$

which finishes the proof of Lemma 7 and hence the proof of Theorem 1. □

II. LOCALITY OF LOCAL ADIABATIC CHANGE

We show in this section that G_n and $\tilde{G}_n$, as defined in Eq. (7) and in Eq. (12) in the main text, generate basically the same dynamics. The proof relies on $\tilde{G}(0)$ being frustration-free, and a runtime of $\tau = O(\log^{1+\alpha}(N/\varepsilon))$, because it turns out that the achieved locality scales linearly with the runtime. We also use the Lieb-Robinson bound [5–8], which states that if H is a local (possibly time-dependent) Hamiltonian with uniformly bounded interaction strengths, $U(t)$ is the unitary evolution generated by H, and O_A, O_B are operators supported on regions A, B, respectively, then

$$\|[U(t)O_A U^\dagger(t), O_B]\| \leq c\min(|A|,|B|)\|O_A\|\|O_B\| \exp\left(\gamma t - \nu L\right), \tag{69}$$

where L is the distance between A and B, and c, γ, ν are constants depending only on the geometry of the lattice and the maximum interaction strength.

The following theorem justifies the replacement of (12) with (7) in the main text, without significantly altering the evolution and thus the final state.

Theorem 8. *Let* $\tilde{G}(s) = \sum_{\mu\in\Upsilon} G_\mu(s)$ *be a frustration-free Hamiltonian path with* $O(N)$ *local terms such that* $|\operatorname{supp}\frac{\mathrm{d}}{\mathrm{d}s}\tilde{G}| = O(1)$*, and let* G *be a localised version of* $\tilde{G}$*, i.e.,*

$$G(s) = \sum_{\mu\in\Upsilon'} G_\mu(s), \quad \Upsilon' = \left\{ \mu \in \Upsilon \mid d\Big(\operatorname{supp}\frac{\mathrm{d}}{\mathrm{d}s}\tilde{G}, \operatorname{supp} G_\mu \Big) < \chi\tau \right\} \tag{70}$$

for some constant χ *and adiabatic runtime* τ*. Let* ψ *and* $\tilde{\psi}$ *be the evolved states under* G *and* $\tilde{G}$ *respectively, i.e.,*

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = G\left(\frac{t}{\tau}\right)\psi(t), \quad i\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\psi}(t) = \tilde{G}\left(\frac{t}{\tau}\right)\tilde{\psi}(t), \quad t\in[0,\tau], \quad \psi(0) = \tilde{\psi}(0) = \phi(0), \tag{71}$$

where $\phi(0)$ *is the ground state of* $\tilde{G}(0)$*. Then, for sufficiently large* $\chi = O(1)$*,*

$$\|\tilde{\psi}(\tau) - \psi(\tau)\| \leq cN^2\tau^2 e^{(\gamma - v\chi/2)\tau}, \tag{72}$$

where c, γ, v *are the constants from* (69)*. In particular, if* $\tau = O(\log^{1+\alpha}(N/\varepsilon))$*, then*

$$\|\tilde{\psi}(\tau) - \psi(\tau)\| \leq \varepsilon/N \tag{73}$$

for sufficiently large $\chi = O(1)$*.*

Proof. For any $\Omega \subseteq \Upsilon$, let $G_\Omega = \sum_{\mu\in\Omega} G_\mu$ and $U_\Omega(t,s)$ be the unitary dynamics generated by G_Ω. Then U_Ω satisfies

$$\partial_t U_\Omega(t,s) = -iG_\Omega(t/\tau)U_\Omega(t,s), \tag{74}$$
$$\partial_s U_\Omega(t,s) = -iU_\Omega(t,s)G_\Omega(s/\tau), \tag{75}$$
$$U_\Omega(t,s) = \mathcal{T}\exp\left\{-i\int_s^t dt' G_\Omega(t'/\tau)\right\}. \tag{76}$$

Notice that $G_{\Upsilon'} = G$ and $G_\Upsilon = \tilde{G}$. We write $U = U_{\Upsilon'}$ and $\tilde{U} = U_\Upsilon$. Let B be the boundary of Υ', that is, $B = \{\mu \in \Upsilon \mid d(\lambda,\mu) = \lceil\chi\tau\rceil\}$ and $\bar{B} = \Upsilon\backslash B$. Then, since $\tilde{G}(0)$ is frustration-free and all terms outside of Υ' are constant, $U_{\bar{B}}(t,0)\phi(0) = U(t,0)\phi(0)$ as $U_{\bar{B}} = U \otimes U_{\bar{B}\backslash\Upsilon'}$ and $U_{\bar{B}\backslash\Upsilon'}\phi(0) = \phi(0)$. In other words, $G_{\bar{B}}$ generates the same dynamics as G. Thus,

$$\|\tilde{\psi}(\tau) - \psi(\tau)\| = \|\tilde{U}\phi(0) - U\phi(0)\| = \|\tilde{U}\phi(0) - U_{\bar{B}}\phi(0)\| = \|\phi(0) - \tilde{U}^\dagger U_{\bar{B}}\phi(0)\|, \tag{77}$$

where $\tilde{U}$ and $U_{\bar{B}}$ are evaluated at $(\tau,0)$. Let $V(t) = \tilde{U}^\dagger(t,0)U_{\bar{B}}(t,0)$. Then, since $G_B = \tilde{G} - G_{\bar{B}}$, Eq. (74) implies

$$\frac{\mathrm{d}}{\mathrm{d}t}V = i\tilde{U}^\dagger(t,0)G_B(t/\tau)\tilde{U}(t,0)V(t). \tag{78}$$

We now approximate V with a local unitary to obtain a bound for (77). Let $X = \{\mu \in \Upsilon \mid d(\mu,B) \le r\}$ for some r to be specified below, and let

$$V_X(t) = \mathcal{T}\exp\left\{i\int_0^t dt' U_X^\dagger(t',0)G_B(t'/\tau)U_X(t',0)\right\} \tag{79}$$

For $r = \frac{1}{2}\chi\tau$ and sufficiently large $\chi = O(1)$, X and $\operatorname{supp}\dot{G}$ are disjoint since $|\operatorname{supp}\dot{G}| = O(1)$, so $G_X(t/\tau) = G_X(0)$ for all $t \in [0,\tau]$. Because of frustration-freeness, $G_X(t/\tau)\phi(0) = 0$, and thus the dynamics generated by G_X acts trivially on the initial state, i.e., $U_X(t,0)\phi(0) = \phi(0)$. Thus, V_X also acts trivially on the initial state, $V_X(t)\phi(0) = \phi(0)$. Hence, substituting this into Eq. (77), we get

$$\|\phi(0) - \tilde{U}^\dagger U\phi(0)\| = \|V_X\phi(0) - \tilde{U}^\dagger U_{\bar{B}}\phi(0)\| = \|\phi(0) - V_X^\dagger V\phi(0)\|. \tag{80}$$

From the definition of V and of V_X,

$$\frac{d}{dt}(V_X^\dagger V) = iV_X^\dagger(\tilde{U}^\dagger G_B\tilde{U} - U_X^\dagger G_B U_X)V, \tag{81}$$

where G_B is evaluated at t/τ. Thus, by integrating (81) and using the triangle inequality and unitary invariance of the operator norm,

$$\|\phi(0) - V_X^\dagger V\phi(0)\| \le \int_0^\tau \mathrm{d}t\|\tilde{U}^\dagger G_B\tilde{U} - U_X^\dagger G_B U_X\| = \int_0^\tau \mathrm{d}t\|G_B - \tilde{U}U_X^\dagger G_B U_X\tilde{U}^\dagger\|, \tag{82}$$

where the unitary evolutions are taken from 0 to t and G_B is evaluated at t/τ. Observe that

$$\partial_s\left(\tilde{U}(t,s)U_X^\dagger(t,s)\right) = -i\tilde{U}(t,s)G_{\bar{X}}(s/\tau)U_X^\dagger(t,s), \tag{83}$$

where $\bar{X} = \Upsilon\backslash X$. Integrating (83) over s, we get

$$G_B(t/\tau) - \tilde{U}U_X^\dagger G_B(t/\tau)U_X\tilde{U}^\dagger = -i\int_0^t \mathrm{d}s\tilde{U}(t,s)\left[G_{\bar{X}}(s/\tau), U_X^\dagger(t,s)G_B(t/\tau)U_X(t,s)\right]\tilde{U}^\dagger(t,s). \tag{84}$$

Therefore, using the triangle inequality and the unitary invariance of the norm, we get

$$\|\psi(\tau) - \tilde{\psi}(\tau)\| \le \int_0^\tau \mathrm{d}t\int_0^t \mathrm{d}s\left\|\left[U_X^\dagger(t,s)G_B(t/\tau)U_X(t,s), G_{\bar{X}}(s/\tau)\right]\right\| \tag{85}$$
$$\le \int_0^\tau \mathrm{d}t\int_0^t ds\ cN^2e^{\gamma(t-s)-\nu r} \le cN^2\tau^2e^{\gamma\tau-\nu r}, \tag{86}$$

where the second line follows from the Lieb-Robinson bound as B and $\bar{X}$ are separated by a distance $r = \frac{1}{2}\chi\tau$. This proves Theorem 8. □

III. RELAXATIONS ON THE ASSUMPTION OF A UNIFORM GAP ALONG THE PATH

In this section, we show that the assumption of a spectral gap along the entire path of $\tilde{G}_n$ can be relaxed.

Theorem 9. *Suppose that $\tilde{G}_n(0)$ has a spectral gap of at least $\delta > 0$. Then $\tilde{G}_n(s)$ has a spectral gap of at least $q_0^2\delta$ for all $s \in [0,1]$, where q_0 satisfies that $\mathbb{1} \geq Q_\lambda \geq q_0\mathbb{1}$ (with Q_λ as in Eq. (3) in the main text). In particular, a uniform gap as defined in the main text implies a constantly lower bounded gap along the entire Hamiltonian path in the given algorithm.*

Proof. Since $\tilde{G}_n(0)$ is positive semidefinite and has a non-trivial kernel, the spectral gap condition of $\tilde{G}_n(0)$ is equivalent to $G_n(0)^2 \geq \delta G_n(0)$. Note that $\mathbb{1} \geq A_{n,m}(s) \geq q_0\mathbb{1}$ (with $A_{n,m}$ as in Eq. (9)). Let $X_n(s) = q_0^2 A_{n,n}^{-1}(s)\tilde{G}_n(0)A_{n,n}^{-1}(s)$. Then,

$$\tilde{G}_n(s) = \sum_{\mu\in\Upsilon}\left(\prod_{m:\lambda_m\in\Lambda_\mu} A_{n,m}^{-1}(s)\right) P_\mu \left(\prod_{m:\lambda_m\in\Lambda_\mu} A_{n,m}^{-1}(s)\right) \tag{87}$$

$$\geq q_0^2 A_{n,n}^{-1}(s)\sum_{\mu\in\Upsilon}\left(\prod_{\substack{m:\lambda_m\in\Lambda_\mu\\ m\neq n}} A_{n,m}^{-1}(s)\right) P_\mu \left(\prod_{\substack{m:\lambda_m\in\Lambda_\mu\\ m\neq n}} A_{n,m}^{-1}(s)\right) A_{n,n}^{-1}(s) \tag{88}$$

$$= q_0^2 A_{n,n}^{-1}(s)\tilde{G}_n(0)A_{n,n}^{-1}(s) \tag{89}$$

$$= X_n(s), \tag{90}$$

where we used in the second line $\|A_{n,n}^{-1}(s)\| \leq q_0^{-1}$. Notice that $\tilde{G}_n(s)$ and $X_n(s)$ have the same kernel and are both positive semidefinite. Thus, the gap of $\tilde{G}_n(s)$ is lower bounded by the gap of $X_n(s)$. But since $G_n(0)^2 \geq \delta G_n(0)$, we also have $X_n(s)^2 \geq q_0^2\delta X_n(s)$ since $A_{n,n}^{-2}(s) \geq \mathbb{1}$. Thus, $\tilde{G}_n(s)$ has a spectral gap of at least $\Delta_n \geq q_0^2\delta$. □

IV. GIBBS STATE PREPARATION IN THE NON-COMMUTING CASE FOR HIGH TEMPERATURES

The algorithm we presented to prepare a purifiaction of the Gibbs state of a Hamiltonian used explicitly that the Hamiltonian is a sum of commuting terms. Thus, one may wonder if one can apply it directly to Gibbs states of non-commuting Hamiltonians H. The genaral answer is no. The reason is that even though a parent Hamiltonian can still be defined as

$$G^{nl}(\beta) = \sum_{\mu\in\Upsilon} G_\mu^{nl}(\beta) = \sum_{\mu\in\Upsilon} e^{\frac{\beta}{2}H} P_\mu e^{-\beta H} P_\mu e^{\frac{\beta}{2}H}, \tag{91}$$

now the terms are not local (hence the superscript nl), and the norm of each term may be exponentially large in N. Thus, adiabatic state preparation using (91) directly takes exponential time. However, in this section we show that for sufficiently high, but constant temperatures, one can approximate G^{nl} by an $r = O(\log N)$-local Hamiltonian G^r which is a sum of $O(\text{poly}(N))$ terms. We also show that in this case, G^{nl} (and thus also G^r) has a $\Omega(1)$ spectral gap and $O(N)$ norm. Because of the existence of the gap, the ground state of G^r is a good approximation of the ground state of G^{nl}.

Using the adiabatic theorem, the following algorithm runs in $O(\text{poly}(N))$ time for high enough (but $\Omega(1)$) temperatures and gives a good approximation of the purification of the Gibbs state of a non-commuting Hamiltonian:

1. Prepare the ground state of $G^r(0) = \sum_{\mu\in\Upsilon} P_\mu$
2. Calculate $G^r(\beta)$
3. Prepare adiabatically the ground state of $G^r(\beta)$

We first use the cluster expansion [9] to construct the approximating Hamiltonian G^r. We also show that the norm of G^{nl} is $O(N)$. Finally, we show that the gap of G^{nl} is $\Omega(1)$. For simplicity, assume that $H = \sum_{\lambda\in\Lambda}$ is a sum of nearest-neighbour interactions, although the results and proofs generalise to other types of interactions. We also assume that $\|h_\lambda\| \leq 1$.

Cluster expansion. We now show that G^{nl} can be approximated by an $r = O(\log N)$-local Hamiltonian G^r. More precisely, we show the following result.

Theorem 10. *For sufficiently small (but constant) β, there exists an $r = O(\log N)$-local Hamiltonian G^r with $O(\mathrm{poly}(N))$ terms such that*

$$\|G^{nl} - G^r\| < O(1/\mathrm{poly}(N)). \tag{92}$$

Moreover, the terms of G^r can be calculated in $O(\mathrm{poly}(N))$ time.

For any function f defined on the subsets of Λ, define the *Möbius transformations*

$$\hat{f}(\Omega) := \sum_{\Theta \subseteq \Omega} f(\Theta), \tag{93}$$

$$\check{f}(\Omega) := \sum_{\Theta \subseteq \Omega} (-1)^{|\Omega \setminus \Theta|} f(\Theta). \tag{94}$$

It is straightforward to check that the following Lemma holds [10].

Lemma 11 (Möbius inversion)**.**

$$\hat{\check{f}} = \check{\hat{f}} = f. \tag{95}$$

For any $\Omega \subseteq \Lambda$, let $H_\Omega = \sum_{\lambda \in \Omega} h_\lambda$, and let $f_\mu(\Omega) = e^{\beta H_\Omega} P_\mu e^{-2\beta H_\Omega} P_\mu e^{\beta H_\Omega}$ for any $\mu \in \Upsilon$. Using Lemma 11, one can express G^{nl}_μ as

$$G^{nl}_\mu = f_\mu(\Lambda) = \sum_{\Omega \subseteq \Lambda} \check{f}_\mu(\Omega). \tag{96}$$

This so-called *cluster expansion* has many interesting properties.

Lemma 12. *Let $\mu \in \Upsilon$. If $\Omega \subseteq \Lambda$ is such that μ is disjoint from Ω and $\Theta \subseteq \Lambda$ is disjoint from Ω, then*

$$\check{f}_\mu(\Omega \cup \Theta) = 0. \tag{97}$$

Proof. We have

$$\check{f}_\mu(\Omega \cup \Theta) = \sum_{\Omega' \subseteq \Omega, \Theta' \subseteq \Theta} (-1)^{|\Omega \setminus \Omega'|} (-1)^{|\Theta \setminus \Theta'|} e^{\beta H_{\Theta'}} P_\mu e^{-2\beta H_{\Theta'}} P_\mu e^{\beta H_{\Theta'}} = 0, \tag{98}$$

since $H_{\Omega'}$ commutes with P_μ and with $H_{\Theta'}$, and the sum over Ω' is 0. □

Lemma 12 states that $\check{f}_\mu$ is non-zero only for connected sets of edges that, in addition, contain μ. Another interesting property of $\check{f}_\mu$ is that its norm can be bounded as follows.

Lemma 13. *For any $\Omega \subset \Lambda$ and any edge μ,*

$$\|\check{f}_\mu(\Omega)\| \leq (e^{4\beta} - 1)^{|\Omega|}. \tag{99}$$

Proof. Expanding the exponentials, one gets

$$\check{f}_\mu(\Omega) = \sum_{\Theta \subseteq \Omega} (-1)^{|\Omega \setminus \Theta|} \sum_{w_1, w_2, w_3 \in \Theta^*} \frac{(-\beta)^{|w_1|} \cdot (2\beta)^{|w_2|} \cdot (-\beta)^{|w_3|}}{|w_1|! \cdot |w_2|! \cdot |w_3|!} h_{w_1} P_\mu h_{w_2} P_\mu h_{w_3}, \tag{100}$$

where Θ^* is the set of all finite sequences of elements of Θ, and for any $w \in \Theta^*$, $|w|$ denotes the length of w and $h_w = h_{\lambda_1} \dots h_{\lambda_{|w|}}$ if $w = (\lambda_1, \dots, \lambda_{|w|})$.

Consider the set $A = \mathrm{supp}(w_1) \cup \mathrm{supp}(w_2) \cup \mathrm{supp}(w_3)$. If $A \neq \Omega$, then the alternating sum in (100) over all Θ such that $A \subseteq \Theta \subseteq \Omega$ is 0. Thus,

$$\|\check{f}_\mu(\Omega)\| \leq \sum_{\substack{w_1, w_2, w_3 \in \Omega^* \\ \mathrm{supp}(w_1) \cup \mathrm{supp}(w_2) \cup \mathrm{supp}(w_3) = \Omega}} \frac{\beta^{|w_1|} \cdot (2\beta)^{|w_2|} \cdot \beta^{|w_3|}}{|w_1|! \cdot |w_2|! \cdot |w_3|!}. \tag{101}$$

But this is exactly a Möbius transform, so

$$\|\check{f}_\mu(\Omega)\| \leq \sum_{\Theta\subseteq\Omega}(-1)^{|\Omega\setminus\Theta|}\sum_{w_1,w_2,w_3\in\Theta^*}\frac{\beta^{|w_1|}\cdot(2\beta)^{|w_2|}\cdot\beta^{|w_3|}}{|w_1|!\cdot|w_2|!\cdot|w_3|!} = \sum_{\Theta\subseteq\Omega}(-1)^{|\Omega\setminus\Theta|}e^{4\beta|\Theta|} = (e^{4\beta}-1)^{|\Omega|}. \tag{102}$$

□

We are now in a position to prove Theorem 10.

Proof of Theorem 10. Using (96), we can write G^{nl}_μ as a sum of local terms where the norm of the terms decay exponentially with their support. As the number of terms with a given size is bounded by the lattice growth constant [11], $\|G^{nl}_\mu\| = O(1)$ above some temperature. Indeed, let η be the lattice growth constant, so that the number of sets of connected edges containing μ and of size M is bounded by $e^{\eta M}$. Then,

$$\|G^{nl}_\mu\| \leq \sum_{\Omega\subseteq\Lambda}\|\check{f}_\mu(\Omega)\| \leq \sum_{M\geq 0}e^{\eta M}(e^{4\beta}-1)^M = O(1) \tag{103}$$

if β is sufficiently small (but constant). In this case, G^{nl}_μ can be approximated by an r-local operator G^r_μ by omitting all connected sets Ω of size at least r. The error of this approximation is

$$\|G^{nl}_\mu - G^r_\mu\| \leq \sum_{|\Omega|\geq r}\|\check{f}_\mu(\Omega)\| \leq \sum_{M\geq r}e^{\eta M}(e^{4\beta}-1)^M = \frac{\left(e^\eta\left(e^{4\beta}-1\right)\right)^r}{1-e^\eta\left(e^{4\beta}-1\right)} = \frac{y^r}{1-y}, \tag{104}$$

where $y = e^\eta\left(e^{4\beta}-1\right)$. Therefore, above some constant temperature, the cluster expansion can be truncated at $|\Omega| \leq O(\log N)$, giving an error of $O(1/\operatorname{poly}(N))$. This results in a $O(\log(N))$-local Hamiltonian

$$G^r = \sum_\mu\sum_{|\Omega|\leq O(\log N)}\check{f}_\mu(\Omega) \tag{105}$$

with $O(\operatorname{poly}(N))$ terms. Note that this Hamiltonian can now be calculated in $O(\operatorname{poly}(N))$ time. Indeed, there are $O(\operatorname{poly}(N))$ terms $\check{f}_\mu(\Omega)$, and each term can be evaluated in $O(\operatorname{poly}(N))$ time since there are at most $O(\operatorname{poly}(N))$ subsets of each Ω. □

Gap of G^{nl}. It remains to be shown that at sufficiently high (but constant) temperatures, the parent Hamiltonian is gapped.

Theorem 14. *For sufficiently small (but constant) β, G^{nl} has a spectral gap of $\Omega(1)$.*

Proof. To show the existence of a gap, we use that $G^{nl} \geq 0$ is frustration-free, so it is enough to show that

$$(G^{nl})^2 \geq \Delta G^{nl} \tag{106}$$

for some $\Delta = \Omega(1)$. Expanding G^{nl}, (106) is equivalent to

$$\sum_\mu (G^{nl}_\mu)^2 + \sum_{\mu\neq\nu}G^{nl}_\mu G^{nl}_\nu \geq \sum_\mu \Delta G^{nl}_\mu. \tag{107}$$

Using Eq. (104) with $r = 1$, we get that G^{nl}_μ is close to $P_\mu = G^{r=1}_\mu$ for high temperatures and thus it is gapped and the gap is close to 1. Therefore, it is enough to show that for some other constant $\Delta' < 1$,

$$\sum_{\mu\neq\nu}G^{nl}_\mu G^{nl}_\nu \geq -\sum_\mu \Delta' G^{nl}_\mu. \tag{108}$$

We upper bound the r.h.s. by lower bounding $\sum_\mu G^{nl}_\mu$ as

$$\sum_\mu G^{nl}_\mu \geq \frac{1}{x}\sum_r e^{-r}\sum_{d(\mu,\nu)=r}G^{nl}_\mu + G^{nl}_\nu, \tag{109}$$

where $x = 2\sum_r e^{-r} C_d r^d = O(1)$ is the number of times a single term is counted, and d is the dimension of the lattice. Therefore, it is enough to prove that for a given r and any pair μ, ν with $d(\mu,\nu) = r$,

$$G_\mu^{nl} G_\nu^{nl} \geq -\Delta' \frac{1}{x} e^{-r} (G_\mu^{nl} + G_\nu^{nl}). \tag{110}$$

Note that the kernel of the LHS of (110) is contained in the kernel of the RHS. Next, $G_\mu^{nl} + G_\nu^{nl}$ can be lower bounded by

$$G_\mu^{nl} + G_\nu^{nl} \geq \frac{1}{2}\left(1 - P_{Ker(G_\mu^{nl} + G_\nu^{nl})}\right), \tag{111}$$

since $G_\mu^{nl} + G_\nu^{nl} \approx P_\mu + P_\nu$, which has gap 1, and at sufficiently high (but constant) temperature the difference is sufficiently small.

To lower bound the l.h.s of (110), write $G_\mu^{nl} = \left|G_\mu^{\lceil r/2 \rceil}\right| + X_\mu$ and $G_\nu^{nl} = \left|G_\nu^{\lceil r/2 \rceil}\right| + X_\nu$. $\left|G_\nu^{\lceil r/2 \rceil}\right|$ and $\left|G_\mu^{\lceil r/2 \rceil}\right|$ commute as they are supported on two disjoint regions, and they are positive, thus their product is also positive. The norm of X_μ, X_ν is bounded by (with $y = e^\eta \left(e^{4\beta} - 1\right)$ as defined in the proof of Theorem 10)

$$\|X_\mu\| = \|G_\mu - |G_\mu^{\lceil r/2 \rceil}|\| \leq \|G_\mu - G_\mu^{\lceil r/2 \rceil}\| + \|G_\mu^{\lceil r/2 \rceil} - |G_\mu^{\lceil r/2 \rceil}|\| \leq 3\frac{y^{\lceil r/2 \rceil}}{1-y}, \tag{112}$$

since $\|G_\nu^{nl} - G_\nu^{\lceil r/2 \rceil}\| \leq y^{\lceil r/2 \rceil}/(1-y)$ by (104), and thus $G_\nu^{\lceil r/2 \rceil} \geq -y^{\lceil r/2 \rceil}/(1-y)$, so $\left|G_\nu^{\lceil r/2 \rceil} - |G_\nu^{\lceil r/2 \rceil}|\right| \leq 2y^{\lceil r/2 \rceil}/(1-y)$. Using that above some constant temperature $\|G_\mu^r\| < 2$, we get that

$$\left\|G_\mu^{nl} G_\nu^{nl} - |G_\mu^{\lceil r/2 \rceil}||G_\nu^{\lceil r/2 \rceil}|\right\| \leq 18\frac{y^{\lceil r/2 \rceil}}{1-y} \leq \Delta' \frac{1}{2x} e^{-r} \tag{113}$$

for sufficiently small (but constant) β. Therefore for any μ, ν pair, the following is true:

$$G_\mu^{nl} G_\nu^{nl} \geq -18\frac{y^{\lceil r/2 \rceil}}{1-y}[1 - P_{Ker(G_\mu^{nl} G_\nu^{nl})}] \geq -\Delta' \frac{1}{2x} e^{-r}[1 - P_{Ker(G_\mu^{nl} + G_\nu^{nl})}] \geq -\Delta' \frac{1}{x} e^{-r}(G_\mu^{nl} + G_\nu^{nl}), \tag{114}$$

as the kernel of $G_\mu^{nl} G_\nu^{nl}$ contains the kernel of $G_\mu^{nl} + G_\nu^{nl}$. This proves Eq. (110) and thus Theorem 14. □

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3.3 Semi-injective PEPS

In this Section, we include the following paper:

- Andras Molnar, Yimin Ge, Norbert Schuch, and J. Ignacio Cirac. "A generalization of the injectivity condition for Projected Entangled Pair States". In: *J. Math. Phys. 59, 021902 (2018)* 59.2, 021902 (June 22, 2017), p. 021902. arXiv: 1706.07329v1

In this project we introduce the class of semi-injective PEPS that encompasses a large set of important states, such as injective PEPS, the two-dimensional AKLT model or the cluster state. We derive a fundamental theorem for them: a way to decide whether two such PEPS describe the same state. The motivation initiates from the understanding of how Gibbs states of commuting local Hamiltonians can be written as PEPS (see Section 3.2). Consider a nearest neighbor Hamiltonian,

$$H = \sum_{\langle ij \rangle} h_{ij}, \tag{3.1}$$

with commuting terms: $[h_{ij}, h_{jk}] = 0$; then, the Gibbs state is simply the product of the local terms:

$$e^{-\beta H} = \prod_{\langle ij \rangle} e^{-\beta h_{ij}}. \tag{3.2}$$

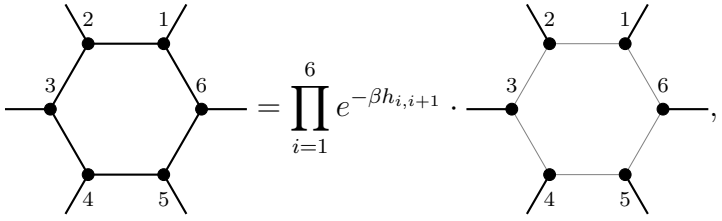
Let us take a Schmidt decomposition of these local operators,

$$e^{-\beta h_{ij}} = \sum_k O_k^{(i)} \otimes O_k^{(j)}. \tag{3.3}$$

The PEPS tensor can then be written as

$$A_{\alpha\beta\gamma\delta} = O_\alpha^{(i)} O_\beta^{(i)} O_\gamma^{(i)} O_\delta^{(i)}. \tag{3.4}$$

Note that operators $O_\alpha^{(i)}$, resulting from the Schmidt decomposition, commute with each other. These PEPS behave similarly to an injective PEPS: they have a parent Hamiltonian with a unique ground state for any finite system size (see Section 3.2). As all classical Hamiltonians are of this form, some of these states are critical, i.e. they have algebraically decaying correlations. In this critical case, the parent Hamiltonian has to be gapless. On a honeycomb lattice, this PEPS is a normal PEPS: grouping the six vertices of a hexagon results in an injective tensor:



where the dots on the l.h.s. represent the PEPS tensors, while those on the r.h.s. – the Schmidt operators $O_\alpha^{(i)}$. Injectivity now follows from the fact that the operator on the r.h.s. is invertible and that the Schmidt vectors are linearly independent. On a square lattice, the same construction is no longer injective. The reason is that in this case, any finite region contains a corner, i.e. a tensor with two edges going out of the region; this results in a non-trivial kernel localized at the corner independent of the size of the region.

This phenomenon does not only occur in case of Gibbs states, but in other important states too, such as the AKLT state in two dimensions, the cluster state, or the CZX model providing a canonical example for SPT order in two dimensions. In this publication, we provide a unified framework for discussing these states by introducing a class of PEPS that we term semi-injective PEPS. We provide a theorem that characterizes when two such PEPS generate the same state, and thus can classify the symmetries of such states. We find that a global symmetry can be represented by an MPO acting on the boundary of a given region. These MPOs provide a (projective) representation of the symmetry group, and the classification of such MPO representations lead to the 3rd cohomology classification of Chen et. al [71]. Therefore the class of semi-injective PEPS provides us with means to rigorously represent the SPT classification in two dimensions.

A generalization of the injectivity condition for Projected Entangled Pair States

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We introduce a family of tensor network states that we term quasi-injective Projected Entangled-Pair States (PEPS). They extend the class of injective PEPS and include other states, like the ground states of the AKLT and the CZX models in square lattices. We construct parent Hamiltonians for which quasi-injective PEPS are unique ground states. We also determine the necessary and sufficient conditions for two tensors to generate the same family of such states in two spatial dimensions. Using this result, we show that the third cohomology labeling of Symmetry Protected Topological phases extends to quasi-injective PEPS.

I. INTRODUCTION

Tensor Network States (TNS) are expected to approximate ground states of local Hamiltonians well[1–3]. Their local description in terms of simple tensors makes them suitable for both numerical and analytical investigations. First, this local structure enables calculations in large or infinite systems. In fact, the Density Matrix Renormalization Group (DMRG) algorithm[4], which proved successful in simulating one-dimensional systems, can be re-expressed in terms of Matrix Product States (MPS)[5,6], the simplest TNS. This connection also motivated a provably efficient algorithm to find the ground state of a gapped one-dimensional local Hamiltonian[7]. Algorithms based on higher-dimensional generalizations of MPS, Projected Entangled Pair States (PEPS[8,9]), are now also giving the best known numerical results for certain Hamiltonians in two dimensions (see, for example, Ref. 10–12). Second, TNS are useful for creating and analyzing exactly solvable models with translation symmetry. Indeed, paradigmatic wavefunctions appearing in different areas of research have a very simple PEPS description, where one can generate a whole family of many-body states by contracting, according to a given geometry, the so-called auxiliary indices of N copies of a single tensor. In two-dimensional systems this includes, for instance, the Cluster State[13,14] underlying measurement based computation, the rotationally invariant spin-liquid AKLT[15,16] and RVB[17] states, and other chiral[18,19] and non-chiral states[20–23] embodying topological order. In particular, PEPS encompass all known non-chiral topological orders[24]. All these states allow for the construction of local parent Hamiltonians and, by making use of their local description, the ground space structure and the behavior of the low-energy excitations can be fully analyzed.

In the last years, the theory of TNS has been considerably developed. In particular, in one dimension a general structural theory of MPS is known. First, the "fundamental theorem of MPS"[25,26] states that any two tensors generating the same family of wavefunctions can always be related by a "gauge" transformation acting on the auxiliary indices of each tensor independently. This result allowed for the classification of symmetry-protected topological (SPT) phases in one dimension[27,28]. Indeed, let us consider an MPS invariant under a symmetry group G. Then, the local gauge transformations which relate the tensor generating the MPS and that obtained by a symmetry action form themselves a *projective* representation of G[29,30]. The equivalence classes formed by those projective representations,

which are labelled by the second group cohomology $H^2(G, U(1))$, thus characterize the different SPT phases under the action of G. Second, for any MPS there exists a systematic way of constructing parent Hamiltonians with a controlled ground space[25,31,32]. All this renders MPS a general framework for the study of solvable models and the classification of phases in one dimension.

In two dimensions, considerable progress has been made in understanding the description of topologically ordered phases in the PEPS framework[20–23,33,34]. However, a general structural theory of PEPS and, in particular, a "fundamental theorem of PEPS", is only known for a specific class, termed "injective"[31,35]. Those are PEPS whose generating tensor, when considered as a map from the auxiliary to the physical indices, can be inverted. While formally, any random PEPS (after blocking few spins) is injective, many relevant examples such as the square lattice AKLT model[16], the RVB[36,37] state, wavefunctions obtained from classical statistical mechanics models[37], as well as all topologically ordered states, do not have this property. Their lack of injectivity prevents us from understanding their behavior under symmetries and, at the same time, makes the canonical construction of parent Hamiltonians with unique ground states for injective PEPS inapplicable.

In order to analyze SPT phases in two dimensions, one might thus tentatively restrict to injective PEPS and apply the fundamental theorem, which yet again yields a projective local symmetry action on the auxiliary indices. However, in two dimensions the classification of projective representations in terms of group cohomology is not stable under blocking, and thus cannot be used to label phases under symmetries unless translational invariance is imposed[38]. This is remedied by the CZX model proposed by Chen *et al.*[38]. It is made up from a *non-injective* PEPS with a corresponding symmetry action, in a way that it exhibits non-trivial symmetry invariants which are insensitive to blocking. Specifically, the symmetry action on the auxiliary indices at the boundary of any region is given by Matrix Product Unitary Operators (MPUOs). Those can be labeled by elements of the third cohomology group $H^3(G, U(1))$ of the symmetry group G, and therefore those elements are expected to label the different SPT phases.

In this paper, we introduce *quasi-injective* PEPS and develop the structure theory for them. They significantly generalize injective PEPS and include, among others, the square-lattice AKLT model, all wavefunctions based on classical models, as well as CZX-like states. Our central result is a "fundamental theorem of quasi-injective PEPS" which states that any

two tensors generating the same quasi-injective PEPS are related by an invertible Matrix Product Operator (MPO) acting on their auxiliary indices. For quasi-injective PEPS with an on-site symmetry, the corresponding MPOs form a representation of the group. We give a general and fully rigorous proof, based on the arguments of Chen *et al.*[38], that these MPO representations are labeled by the third cohomology group $H^3(G, \mathbb{C}^*) = H^3(G, U(1))$, suggesting that this labels SPT phases for all quasi-injective PEPS, including those away from fixed point wavefunctions[39] or with non-unitary symmetries. We further show that symmetries of quasi-injective PEPS must have a special two-layer structure. This, by itself, enables the definition of an MPO acting on the physical indices alone, and thus allows one to assign another label $H^3(G, \mathbb{C}^*)$ to the symmetry action, which we show to coincide with that of the MPO acting on the boundary. Therefore, the SPT labeling is just as much a property of the physical symmetry itself as it is of the boundary, and can in fact be directly inferred by analyzing the structure of the physical symmetry action, without needing to invoke the underlying PEPS. As a corollary, this implies that the H^3 label of the MPO action is well-defined and, in particular, the same on the horizontal and vertical boundaries, also in the absence of rotational symmetry. Furthermore, we also provide two different construction for parent Hamiltonians with unique ground states.

The paper is structured as follows. In Section II we introduce the formalism, and define quasi-injective PEPS. In Section III, we give an overview of the main results of the paper. Readers who are interested only in the results rather than the proofs might thus restrict to Sections II and III. In Section IV, we discuss parent Hamiltonian for quasi-injective PEPS. In Section V, we summarize central results from the structure theory of MPS needed for the remainder of the paper. In Section VI, we develop the structure theory of quasi-injective PEPS, i.e., we give a local characterization of when two quasi-injective PEPS generate the same state. In Section VII, we apply this to characterize symmetric quasi-injective PEPS, yielding the characterization in terms of the third cohomology group.

II. FORMALISM

In this section we introduce MPS, PEPS and the graphical calculus commonly used in the field of tensor networks (TNs). We modify the standard notations in order to be able to represent TNs that are concatenations of several layers of two-dimensional TNS. Using

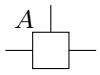
this notation, we define quasi-injective PEPS. We show that this class of PEPS contains all injective PEPS as well as some examples that are not known to have injective PEPS description.

A. Notation

Translationally invariant MPS are defined in terms of a single rank-three tensor $A \in \mathbb{C}^D \otimes \mathbb{C}^D \otimes \mathbb{C}^d$, $A = \sum_{\alpha,\beta,i} A^i_{\alpha\beta} |\alpha\rangle\langle\beta| \otimes |i\rangle = \sum_i A^i \otimes |i\rangle$. The corresponding state on n particles is

$$|V_n(A)\rangle = \sum_i \mathrm{Tr}\{A^{i_1} \dots A^{i_n}\} |i_1 \dots i_n\rangle \ . \tag{1}$$

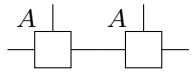
The tensor and the corresponding state can be represented graphically as follows. Each tensor is represented with a square with lines attached to it. The number of lines connected to the rectangle is the rank of the tensor and each line represents one index. For example, the single MPS tensor is represented as:



(2)

Tensor contractions are depicted by joining the lines corresponding to the indices contracted. For example, the contraction of two MPS tensors is

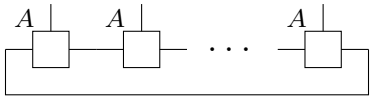
$$\sum_{\alpha\beta\gamma ij} A^i_{\alpha\beta} A^j_{\beta\gamma} |\alpha\rangle\langle\gamma| \otimes |ij\rangle =$$



(3)

Same way, the MPS can be depicted as:

$$|V_n(A)\rangle = \sum_i \mathrm{Tr}\{A^{i_1} \dots A^{i_n}\} |i_1 \dots i_n\rangle =$$

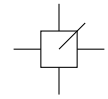


(4)

We refer to the contracted legs as *bonds* or *virtual indices*, D as the *bond dimension* of the MPS tensor A, the uncontracted leg as *physical index*, and d as the *physical dimension* of A.

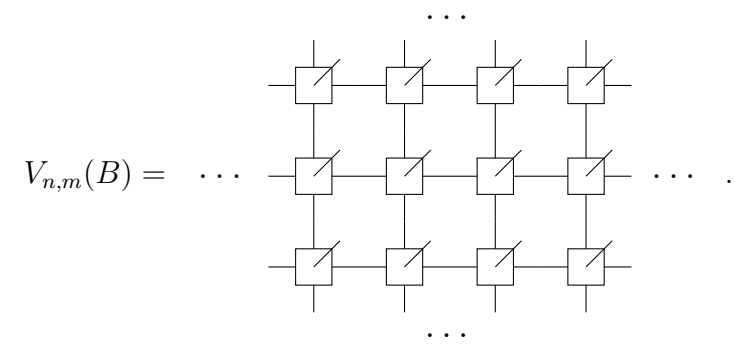
We will define PEPS now as generalizations of MPS. We will consider a square lattice, although other geometries can also be used. Take a rank-five tensor B:

$$B =$$

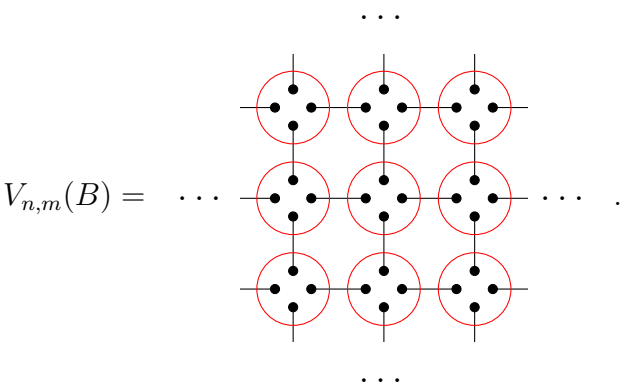


(5)

Consider an $n \times m$ rectangular grid with periodic boundary conditions (that is, on a torus). PEPS is defined then by placing the tensor B at every lattice point and contracting the neighboring tensors:

$V_{n,m}(B) =$  . (6)

An equivalent description is the following. Place maximally entangled pair states on the edges of the grid. These particles are referred to as virtual particles. At every lattice point, act with an operator on the four virtual particles closest to the lattice point:

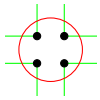
$V_{n,m}(B) =$  . (7)

Here each dot represents a virtual particle, the lines connecting them represent that they are in an entangled (here the maximally entangled) state. The red circles depict the operators acting on the four virtual particles. We call a PEPS *injective* if these operators are injective maps.

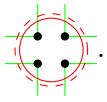
In the following, we use this notation when drawing tensor networks in two dimension. For example, a four-partite state will be depicted as

 . (8)

This four-partite state can equally be thought of as a non-translationally invariant MPS on four sites. Then each corner depicts an MPS tensor. Operators are depicted as circles or rectangles. For example,

 (9)

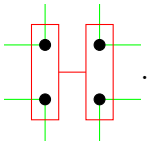
depicts a four-partite operator acting on the physical indices (black points) of four MPS tensors. In certain cases, we need more than two layers of tensors. In this case the upper layer is drawn bigger. For example a product of two operators acting on four MPS tensors are depicted as



(10)

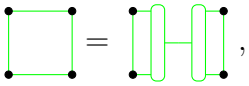
In this case the operator depicted as a solid circle acts first on the four MPS tensors, the dashed one acts second.

We will often use a minimal rank decomposition of tensors. For convenience, we will refer to the operators in the decomposition as Schmidt vectors, even though the minimal rank decomposition is not necessarily a Schmidt decomposition, as we don't require orthogonality. For example, a minimal rank decomposition of a four-partite operator acting on four MPS tensors will be depicted as:



(11)

The Schmidt vectors of a four-partite state $|\phi\rangle$ can be related to its MPS description. We will therefore depict the minimal rank decomposition as



(12)

where the Schmidt vectors are denoted as:

(13)

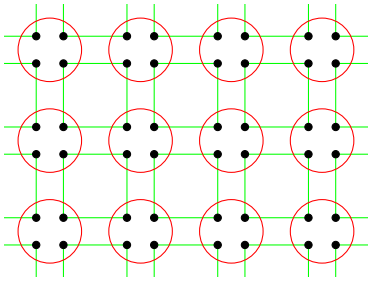
B. Quasi-injective PEPS

In this section we define quasi-injective PEPS. We show that this class contains all injective PEPS. Moreover, we provide examples that are not known to admit an injective PEPS description, yet they can be written as quasi-injective PEPS.

Definition 1 (Quasi-injective PEPS)**.** Let $|\phi\rangle$ be a four-partite state with full rank reduced densities at every site, and let O be an invertible operator. The *quasi-injective* PEPS

$|\Psi_{n\times m}(\phi, O)\rangle$ is defined as

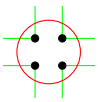
$$|\Psi_{n\times m}(\phi, O)\rangle = \quad , \tag{14}$$



where the green rectangle is $|\phi\rangle$ and the red circle is O, and the state is defined on a torus with $n \times m$ copies of $|\phi\rangle$. We will often drop $|\phi\rangle$ and O and the indices n, m from the notation.

Note that the full rank assumption does not affect which states can be described as quasi-injective PEPS, it is only needed to avoid unnecessary degrees of freedom in the operator O.

These states can be written as a PEPS, but that PEPS is in general not injective. For example, a PEPS tensor generating the same state is

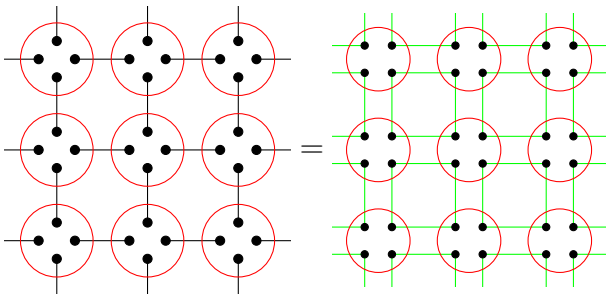


(15)

with an arbitrary (non necessarily translational invariant) MPS decomposition of $|\phi\rangle$.[1]

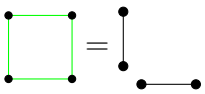
In the following we show that these states include injective PEPS as well as all the examples mentioned above.

a. Injective PEPS. In this case the invertible operator is the PEPS tensor, and the four-partite state consists of two maximally entangled pairs (and a one-dimensional particle):



(16)

where the four-partite states are (the fourth particle is a scalar):



(17)

[1] TN states of this form have been used in other contexts, see e.g. Ref. 40.

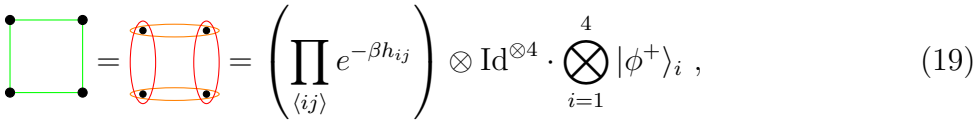
b. The CZX model The CZX model readily admits quasi-injective PEPS form: the four-partite states are GHZ states $|0000\rangle + |1111\rangle$, whereas the invertible operators are unitary operators $U_{CZX} = X^{\otimes 4} \cdot \prod_{\langle ij \rangle} CZ_{ij}$.

c. Purification of thermal states. Consider a commuting nearest neighbor Hamiltonian on a square lattice and the following purification of its Gibbs state:

$$|\Psi\rangle = \frac{1}{\sqrt{Z}} \left(e^{-\beta H/2} \otimes \mathrm{Id}\right) \bigotimes_i |\phi^+\rangle_i \ , \tag{18}$$

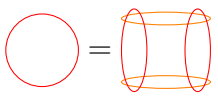
where $|\phi^+\rangle = \sum_j |jj\rangle$ is a maximally entangled pair state, and $e^{-\beta H} \otimes \mathrm{Id}$ acts non-trivially on one of the entangled pairs at every lattice site. This state admits a PEPS description: as the Hamiltonian terms are commuting, $e^{-\beta H/2}$ is a product of local operators. The PEPS tensors are then simply the product of the Schmidt vectors of these local operators acting on $|\phi^+\rangle$. This tensor does not become injective after blocking exactly because of the corners: after blocking, the operators lying entirely inside the blocked region can be inverted. Note that applying invertible operators on the tensor doesn't change injectivity. This factorizes the tensor into a product of tensors on the boundary and tensors on the corners. The boundary is injective, while the corners are not: the Schmidt vectors of the Hamiltonian terms commute, therefore any antisymmetric state on the corner is mapped to zero.

Nevertheless, these states admit a quasi-injective PEPS representation. Indeed, block 2×2 pairs of particles. The four-partite state in the quasi-injective PEPS description consists of the four pairs of particles in the state



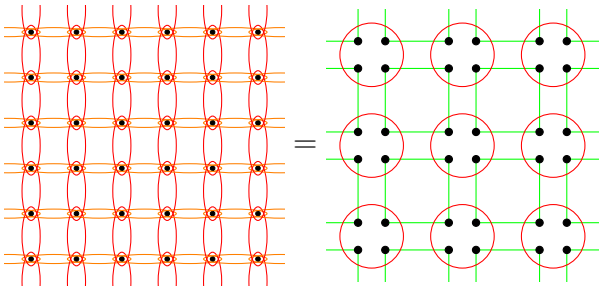
$$= \left(\prod_{\langle ij \rangle} e^{-\beta h_{ij}} \right) \otimes \mathrm{Id}^{\otimes 4} \cdot \bigotimes_{i=1}^{4} |\phi^+\rangle_i \ , \tag{19}$$

where both i and j runs over the particles in one block and $|\phi^+\rangle$ is the maximally entangled state. The dots represent $|\phi^+\rangle$, while the ellipses $e^{-\beta h_{ij}} \otimes \mathrm{Id}^{\otimes 2}$. The invertible operator is a product of $e^{-\beta h_{ij}} \otimes \mathrm{Id}^{\otimes 2}$ on the 2×2 block shifted by half a lattice constant in both directions:



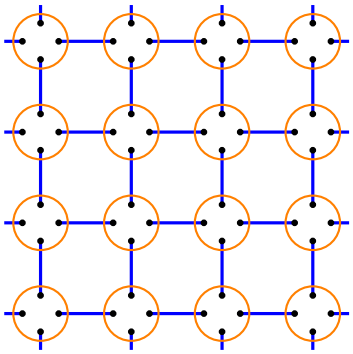
. (20)

With this convention, the state is written as an injective PEPS as follows:



(21)

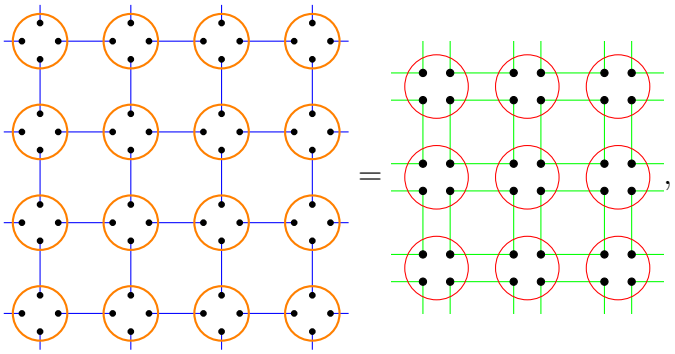
d. AKLT in two dimensions. The two-dimensional AKLT model is a spin-2 system which is constructed as follows: place a singlet $|01\rangle - |10\rangle$ on each edge of a square lattice. Then, at each vertex, project the four virtual qubits into the 5-dimensional symmetric subspace:

$|\Psi_{AKLT}\rangle =$ 

(22)

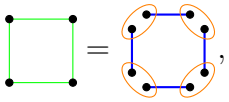
Here the blue lines represent singlets, the orange circles projectors into the symmetric subspace. As any virtual boundary state which is anti-symmetric on the two qubits of any corner is in the kernel of the map after appropriate applications of single-qubit Ys, the PEPS tensors describing this state cannot be injective, even after blocking.

The two-dimensional AKLT admits a quasi-injective PEPS description as follows:



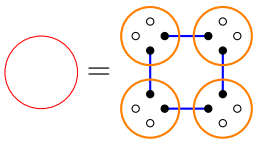
(23)

with the four-partite state



(24)

where the blue lines are singlets, and the orange ellipses are the projectors into the 3-dimensional symmetric subspace (the four-partite state can thus effectively be viewed as a state on four qutrits: the one-dimensional AKLT state on four particles), and



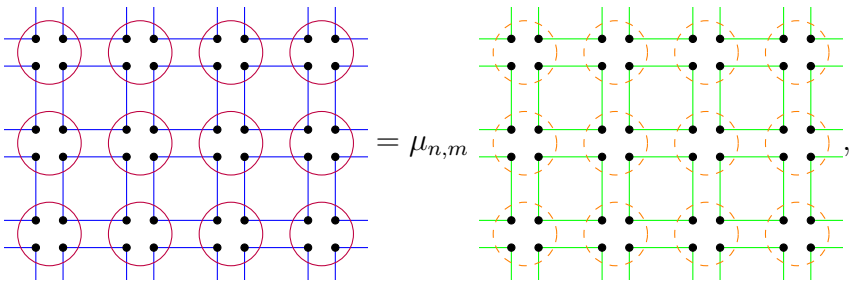
(25)

which acts on the qubits represented by the hollow dots, restricted to the symmetric subspace at each corner. It can be verified that the rank of (25) is 81. Clearly, the image of the adjoint of (25) is contained in the subspace which is symmetric in the pairs of qubits at each corner. The dimension of the latter is also 81. Thus, (25) is invertible.

III. SUMMARY AND RESULTS

In this section, we give a summary of the results obtained in this work. The detailed derivations of all these results are given in the subsequent sections. The results extend the properties known for injective PEPS to quasi-injective ones. First, we show how to construct local Hamiltonians for which they are the unique ground states. Next, we answer the question under which local conditions two quasi-injective PEPS generate the same state. We then use this result to characterize symmetries in quasi-injective PEPS. We also find that the third cohomology classification of SPT phases naturally extends to these states, and thus these states might be suitable to capture the physics of SPT phases. In the following, we give a detailed description of the results.

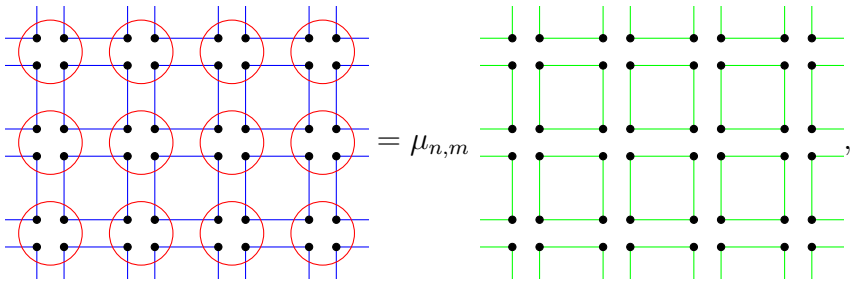
Consider two quasi-injective PEPS generated by (ϕ_A, O_A) and (ϕ_B, O_B). Suppose that on an $n \times m$ torus, they generate states that are proportional to each other:



(26)

where the purple circle and the blue rectangle depicts O_A and $|\phi_A\rangle$, while the orange dashed

circle and the green rectangle depicts O_B and $|\phi_B\rangle$ and $\mu_{n,m} \in \mathbb{C}$. Inverting O_B, we obtain



(27)

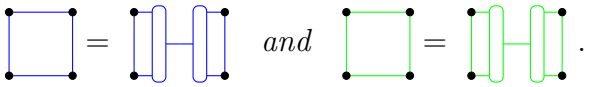
where the red circle denotes the invertible operator $O = O_B^{-1} O_A$.

In this setup, we prove the following:

Theorem 1. *If Eq. (27) holds for some specific $n_0, m_0 \geq 3$, then for all $n, m \in \mathbb{N}$,*

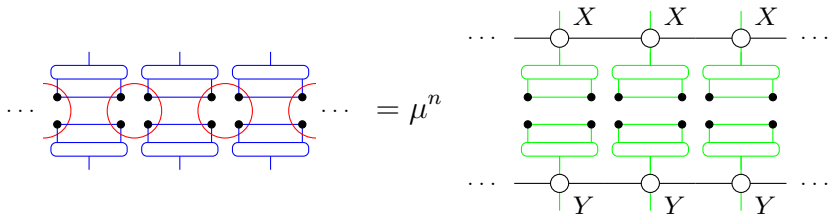
1. *Eq. (27) holds with $\mu_{n,m} = \mu^{nm}$.*

2. *The action of O corresponds to an MPO acting on the boundary as follows: Take a minimal rank decomposition of the four-partite states w.r.t. the vertical cut. That is, write*



(28)

Then for the Schmidt vectors defined as above, the following holds: There are two MPO tensors X and Y such that



(29)

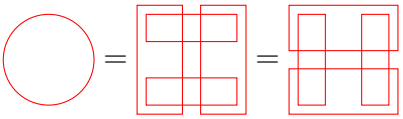
where $\mu \in \mathbb{C}$ is the proportionality constant from Point 1 above, $V_n(Y) = (V_n(X))^{-1}$ for every size n, and both X and Y become injective after blocking two tensors.

3. *The operator O is a four-particle non-translationally invariant MPO with the property that cutting the MPO into two halves yields a minimal rank decomposition of O.*

4. *The operator O is a product of two-body invertible operators:*

$$O = (O_{14} \otimes O_{23}) \cdot (O_{12} \otimes O_{34}) = \left(\tilde{O}_{12} \otimes \tilde{O}_{34}\right) \cdot \left(\tilde{O}_{14} \otimes \tilde{O}_{23}\right) \ , \tag{30}$$

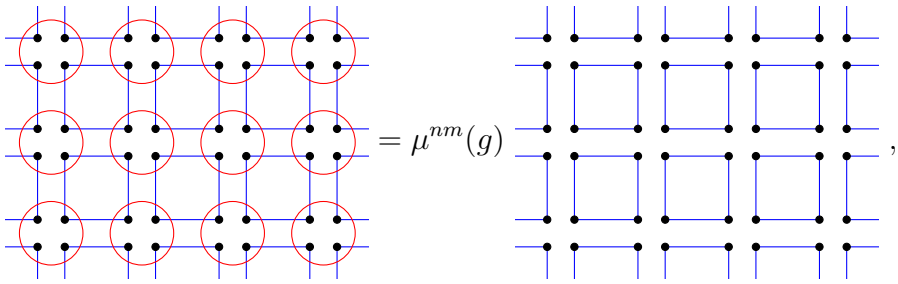
where the particles are numbered clockwise from the upper left corner and O_{ij} acts on particles i and j. Pictorially,



(31)

In Section VII we use these results to rederive the third cohomology classification of SPT phases within the framework of quasi-injective PEPS. The setup in this case is as follows:

Let G be a group, O_g a faithful (not necessarily unitary) representation of G. Let $|\phi\rangle$ be a four-partite state with full rank one-particle reduced densities. Suppose $\forall g \in G$, O_g is a symmetry of the quasi-injective PEPS defined by $|\phi\rangle$ and Id:



(32)

where the blue squares represent $|\phi\rangle$, the red operators O_g.

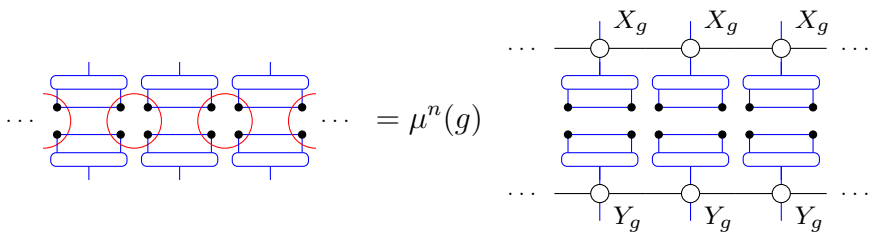
Note that this setup can readily be applied for unitary symmetries of quasi-injective PEPS: let the quasi-injective PEPS be defined by the four-partite state $|\phi\rangle$ and an invertible operator A. Let the unitary representation of the symmetry group G be U_g. Then, by inverting A in the symmetry condition, we arrive to Eq. (32) with $O_g = A^{-1}U_gA$.

Within this setup, we prove that

Theorem 2. *If Eq. (32) holds for some $n, m \geq 3$, then*

1. *$g \mapsto \mu(g)$ is a one-dimensional representation of G.*

2. *For every $g \in G$ there are two MPO tensors X_g and Y_g such that*



(33)

and $V_n(Y_g) = (V_n(X_g))^{-1}$ for all n. Moreover, $V_n(X_g)$ and $V_n(Y_g)$ form projective representations of G with $V_n(X_g)V_n(X_h) = \lambda^n(g,h)V_n(X_gX_h)$ for a two-cocycle λ. In particular, $V_n(X_g)V_n(X_h)$ has only one block in its canonical form.

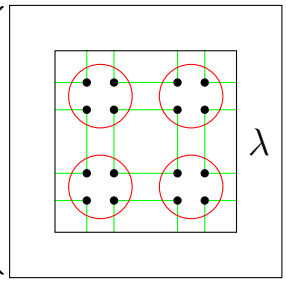
3. *There is a canonical way to assign an element from* $H^3(G, \mathbb{C}^*)$ *to the one-block MPO representation* $g \mapsto X_g$.

4. O_g *has a four-particle non-translationally invariant MPO representation with tensors* $O_g^{(1)}, O_g^{(2)}, O_g^{(3)}, O_g^{(4)}$ *in the sense of Theorem 1, Point 3, such that the MPO* $V_n(O_g^{(1)} O_g^{(2)} O_g^{(3)} O_g^{(4)})$ *forms a one-block projective MPO representation and its cohomology label coincides with that of the boundary. In particular, the MPO labels obtained from the vertical and horizontal boundaries are the same.*

IV. PARENT HAMILTONIAN

In this section, we prove that quasi-injective PEPS are unique ground states of their parent Hamiltonian. Let us consider a quasi-injective PEPS $|\psi\rangle$. Corresponding to this state, we consider two parent Hamiltonian constructions. First, one can obtain the usual parent Hamiltonian by writing the state as a PEPS with the tensors in Eq. (15). That is, consider a 2×2 patch of the tensors. Let S be the subspace generated by the tensors with arbitrary boundary conditions:

$$S = \left\{ \lambda \;\middle|\; \lambda \in \mathbb{C}^{D_v^4 D_h^4} \right\} \tag{34}$$



The Hamiltonian term $\tilde{h}_i$ centered around the plaquette state at position i is just the projector onto $S^\perp$ and the Hamiltonian $\tilde{H}$ is the sum over all positions of these projectors:

$$\tilde{h}_i = \mathrm{Proj}\left(S^\perp\right)_i \otimes \mathrm{Id} \tag{35}$$

$$\tilde{H} = \sum_i \tilde{h}_i. \tag{36}$$

The second construction is to invert the operators O around a plaquette state at site i and project ϕ_i to zero:

$$h_i = \left(\prod_{\langle ji \rangle} O_j^{-1} \right)^\dagger P_i \left(\prod_{\langle ji \rangle} O_j^{-1} \right), \tag{37}$$

where j runs over all positions of operators that (partially) act on the plaquette state at position i and the projector P_i is the projector to the orthocomplement of $\mathbb{C}|\phi\rangle$: $P_i = (\mathrm{Id}_i - |\phi\rangle_i\langle\phi|) \otimes \mathrm{Id}$. Then the Hamiltonian H is the sum of the different terms:

$$H = \sum_i h_i. \tag{38}$$

Proposition 3. *The quasi-injective PEPS $|\psi\rangle$ is the unique ground state of both H and $\tilde{H}$ at all system sizes.*

Proof. We first prove that H has a unique ground state. Then we prove that the kernel of $\tilde{H}$ is contained in that of H.

To see that $\ker H$ is one-dimensional, consider the following similarity transform:

$$\left(\prod_j O_j\right)^\dagger H \left(\prod_j O_j\right) = \sum_i P_i \otimes \mathrm{Id} \otimes \bigotimes_j \left(O_j^{-1}\right)^\dagger O_j^{-1}, \tag{39}$$

where the product runs over all sites j that are not neighbors of the projector P_i, and the identity acts on all virtual particles that are neighbors of the four-partite state $|\phi\rangle$. The kernel of each term in the sum is $|\phi\rangle_i \otimes \bigotimes_{j\notin i} \mathcal{H}_j$, where j runs over all virtual particles that are not in the four-partite state $|\phi\rangle$. Clearly the intersection of these subspaces is $\bigotimes_i |\phi\rangle_i$, that is, the kernel of H is one-dimensional.

To see that $\ker \tilde{H} \leq \ker H$, notice that every state in S_i (defined in Eq. (34)) is in the kernel of h_i. Therefore,

$$\ker \tilde{h}_i \leq \ker h_i. \tag{40}$$

Finally, as $\ker H = \cap_i \ker h_i$ and $\ker \tilde{H} = \cap_i \ker \tilde{h}_i$, the inclusion also holds for the kernel of the total Hamiltonians. □

V. BACKGROUND: MATRIX PRODUCT STATES

In this Section we recall some basic properties of MPS. These definitions and theorems are mainly covered in Ref. 26. First, recall some basic properties of completely positive maps.

Definition 2. A completely positive map $T : \rho \mapsto T(\rho) = \sum_i A_i \rho A_i^\dagger$ is

- *irreducible* if there is no non-trivial projector P such that $T(\rho) = PT(\rho)P^\dagger$ for all $\rho = P\rho P^\dagger$. Otherwise T is reducible.

- *primitive* if $\exists n$ such that $T^n(\rho) > 0$ for all $\rho \geq 0$.

Note that then the following statements hold:

Proposition 4. *Let $T : \rho \mapsto T(\rho) = \sum_i A_i \rho A_i^\dagger$ be a completely positive map with spectral radius r. Then r is an eigenvalue with at least one positive semidefinite eigenvector. Moreover,*

- *T is primitive if and only if r has multiplicity one, the corresponding eigenvector is positive definite, and there are no other eigenvalues of magnitude r.*

- *if T is irreducible but not primitive, then r has multiplicity one, and all eigenvalues of magnitude r are $r \cdot \exp[2\pi i n/K]$ for some K and $n = 1, 2 \ldots K$. We call K the periodicity of T.*

- *T is reducible if and only if $A^i P = P A_i P$ for some non-trivial projector P.*

For proofs, see e.g. Ref. 41 and 42. Now we define Matrix Product States.

Definition 3. An *MPS tensor* is a tensor $A \in \mathbb{C}^D \otimes (\mathbb{C}^D)^* \otimes \mathbb{C}^d$,

$$A = \sum_{i\alpha\beta} A^i_{\alpha\beta} |\alpha\rangle\langle\beta| \otimes |i\rangle = \sum_i A^i \otimes |i\rangle. \tag{41}$$

For any $n \in \mathbb{N}$, the state $V_n(A) \in (\mathbb{C}^d)^{\otimes n}$ is then defined as

$$V_n(A) = \sum_{i_1 \ldots i_n} \mathrm{Tr}\left\{A^{i_1} \ldots A^{i_n}\right\} |i_1 \ldots i_n\rangle. \tag{42}$$

The *transfer matrix* of A, T_A is the completely positive map $T_A : \rho \mapsto \sum_i A_i \rho A_i^\dagger$. We say that A is

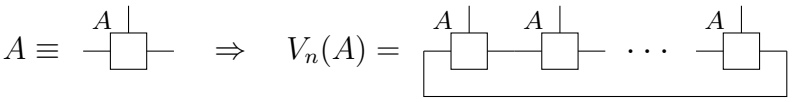
- *injective*, if $\sum_i \mathrm{Tr}\{A^i \rho\}|i\rangle = 0$ implies $\rho = 0$.

- *normal*, if T_A is primitive.

- *periodic*, if T_A is irreducible but not primitive.

An MPS is called *normal, injective or periodic*, if it can be generated by a normal, injective or periodic MPS tensor.

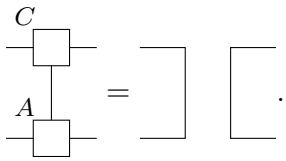
We often depict an MPS tensor and the corresponding MPS as follows:



(43)

The horizontal legs of the MPS tensor A are often referred as the *virtual indices*, while the vertical one as the *physical index* of A. The dimension of the virtual indices, D, is called the *bond dimension* of A.

Note that, unlike in Ref. 26, for convenience, we do not suppose that the spectral radius of a normal tensor is 1. Note also that an MPS tensor is injective if and only if it has a left inverse, C, such that $\sum_i A^i \otimes C^i = \mathrm{Id}$ in the sense as depicted below:



(44)

Here, and in the following, we use the following graphical calculus[43] of tensors. A tensor is depicted as a box or circle, with some lines attached to it. These lines represent the indices of the tensor. Tensor contraction is depicted by joining the lines. In the picture above, for example, we have contracted the physical indices of A and C. The result is the identity tensor from the bottom indices to the top indices. We have omitted drawing a box for the identity.

A frequently used concept in MPS theory is the blocking of tensors.

Definition 4 (Blocking)**.** The MPS tensor B is a *blocking* of A if $B = \sum_{i_1 \dots i_k} A^{i_1} \dots A^{i_k} \otimes |i_1 \dots i_k\rangle$. Note that $V_n(B) = V_{kn}(A)$.

We will often write the above contraction of tensors as a product. That is, for any two MPS tensors C and D, $CD := \sum_{ij} C^i D^j \otimes |ij\rangle$. With this notation, $B = AA \dots A$. We will use this notation even if one of the tensors does not have a physical index.

Note that a normal tensor stays normal after blocking. Moreover, injective and normal MPS are the same up to blocking:

Proposition 5. *Any injective tensor is proportional to a normal tensor. Conversely, for any normal tensor* $\exists L_0 \in \mathbb{N}$ *such that it becomes injective after blocking any* $L \geq L_0$ *tensors. The minimal such* L_0 *is called the injectivity length.*

This statement was proven e.g. in Ref. 44. Note that L_0 might be bigger than the primitivity length of T_A, that is, the minimal n for which $T_A^n(\rho) > 0$ for all $\rho \geq 0$. There is, however, a universal bound depending only on the bond dimension D.

Note that being normal or injective are properties which are stable under taking tensor product of MPS tensors:

Proposition 6. *The tensor product of two normal MPS tensors is normal. The tensor product of two injective MPS tensors is injective.*

Proof. First, we prove that the tensor product of two normal tensors A and B is normal. The transfer matrix of $A \otimes B$ is $T_A \otimes T_B$, where T_A is the transfer matrix of A and T_B is the transfer matrix of B. Denote the spectrum of any operator T by $\sigma(T)$. Then $\sigma(T_A \otimes T_B) = \sigma(T_A) \cdot \sigma(T_B)$. Therefore, $T_A \otimes T_B$ has a unique eigenvalue with magnitude (and value) equal the spectral radius. The corresponding eigenvector of $T_A \otimes T_B$ is $\rho_A \otimes \rho_B$ if ρ_A and ρ_B are the eigenvectors of T_A and T_B with maximum eigenvalue, respectively. $\rho_A \otimes \rho_B$ is positive and is full rank, so $T_A \otimes T_B$ is primitive.

Second, the tensor product of two injective tensors is injective: if A and B are injective and A^{-1} and B^{-1} are their left inverses, then $A^{-1} \otimes B^{-1}$ is a left inverse of $A \otimes B$. □

Proposition 7. *Given two normal tensors A and B with injectivity length at most L, the two MPS generated by them either become perpendicular in the thermodynamic limit, i.e.*

$$\frac{|\langle V_n(A)|V_n(B)\rangle|}{\|V_n(A)\| \cdot \|V_n(B)\|} \to 0 \tag{45}$$

as $n \to \infty$, or the following three equivalent statements hold:

- *$V_n(A) = \lambda^n V_n(B)$ for some $\lambda \in \mathbb{C}$ for all n*
- *$\exists n \geq 2L+1$ such that $V_n(A) = \lambda^n V_n(B)$ for some $\lambda \in \mathbb{C}$*
- *$A^i = \lambda X B^i X^{-1}$, for some $\lambda \in \mathbb{C}$ and this X is unique up to a constant*

We call the normal tensors A and B *essentially different* if the MPSs generated by them are not proportional in the above sense. The proof of these statements can be found in Ref. 26.

Corollary 7.1. *Given a set of pairwise essentially different normal tensors, A_i, $\exists N \in \mathbb{N}$ such that the MPS $V_n(A_i)$ are linearly independent for all $n > N$.*

Proposition 8. *Any MPS $V_n(A)$ can be decomposed into a linear combination of normal and periodic MPSs:*

$$V_n(A) = \sum_i \mu_i^n V_n(A_i), \tag{46}$$

where each A_i is either normal or periodic.

The proof can be found in Ref. 26. We provide a simplified proof here.

Proof. We prove this by induction on the bond dimension D. If $D = 1$, A_i is proportional to a normal MPS. Suppose now that the statement is true for all $D < D_0$. Consider an MPS tensor A with bond dimension D_0. If its transfer matrix T_A is irreducible, then A is either periodic or proportional to a normal MPS tensor. Otherwise, there exists a non-trivial projector P such that $A_i P = P A_i P$, see Proposition 4. Then $V_n(A) = V_n(PAP) + V_n(QAQ)$ with $Q = 1 - P$. Finally, the bond dimension of PAP (and QAQ) can be compressed to the rank of P (corr. Q): write $P = YX$ for some $X : \mathbb{C}^{D_0} \to \mathbb{C}^D$, $Y : \mathbb{C}^D \to \mathbb{C}^{D_0}$, $XY = \mathrm{Id}_D$. Then XAY generates the same MPS as PAP. The bond dimension of the resulting MPS is smaller than D_0, thus by the induction hypothesis, they can be written as a linear combination of normal or periodic MPS. □

Proposition 9. *Let A be a periodic MPS tensor with periodicity K. After blocking K tensors, $V_n(A)$ decomposes into K essentially different normal MPS:*

$$V_{Kn}(A) = \sum_{i=1}^{K} V_n(B_i), \tag{47}$$

where the B_is are pairwise essentially different normal MPS tensors on K spins. Moreover, $V_n(A) = 0$ if $n \notin K\mathbb{N}$.

This statement has been proven as Lemma 5 in Ref. 45. Proposition 9 from Ref. 26 is a corollary of this:

Corollary 9.1. *For any MPS tensor A $\exists K$ such that after blocking K tensors, $V_{Kn}(A)$ decomposes into the following linear combination of normal tensors:*

$$V_{Kn}(A) = \sum_i \left(\sum_j \mu_{ij}^n \right) V_n(B_i), \tag{48}$$

where the B_is are pairwise essentially different normal tensors on K sites.

Finally, the following statement, together with Corollary 7.1, provides the "uniqueness" of this decomposition:

Proposition 10. *If for* $\mu_1, \dots \mu_r \in \mathbb{C}\backslash\{0\}$ *and* $\lambda_1, \dots \lambda_s \in \mathbb{C}\backslash\{0\}$

$$\sum_{i=1}^{r} \mu_i^n = \sum_{j=1}^{s} \lambda_j^n \tag{49}$$

for all $n \in \mathbb{N}$*, then* $r = s$ *and* $\mu_i = \lambda_{p(i)}$ *for some permutation* p *and for all* i *.*

This statement has been proven as Lemma 9 in Ref. 46.

We will also consider non-translationally invariant MPS.

Definition 5. Let d_i and D_i $(i = 1 \dots k)$ be positive integers. Let $X_i = \sum_{j=1}^{d_i} X_i^j \otimes |j\rangle \in \mathbb{C}^{D_i} \otimes \left(\mathbb{C}^{D_{i+1}}\right)^* \otimes \mathbb{C}^{d_i}$ be tensors for $i = 1 \dots k$, where we identify $k+1$ with 1. Then the *non-translationally invariant MPS* defined by these tensors is

$$V(X_1, \dots, X_k) = \sum_{i_1=1}^{d_1} \cdots \sum_{i_k=1}^{d_k} \mathrm{Tr}\left\{X_1^{i_1} \dots X_k^{i_k}\right\} |i_1 \dots i_k\rangle \ . \tag{50}$$

A non-translationally invariant MPS is called *injective after blocking* l *sites* if $\forall i = 1 \dots k$ the tensor $X_i X_{i+1} \dots X_{i+l}$ satisfies that if $\mathrm{Tr}\left\{\rho X_i^{j_1} X_{i+1}^{j_2} \dots X_{i+l-1}^{j_l}\right\} |j_1 \dots j_l\rangle = 0$, then $\rho = 0$.

Proposition 11. *Let* $X_1, \dots X_k$ *define a non-translationally invariant MPS that is injective after blocking* l *sites. Then the MPS is also injective after blocking any* $m \geq l$ *sites.*

Proof. We prove this by induction on m. For $m = l$, the statement is true by assumption. Suppose that the MPS is injective after blocking m tensors. Let $\rho \in \mathbb{C}^{D_{i+m}} \otimes \mathbb{C}^{D_i}$ such that for $m+1$ consecutive sites

$$\sum_{j_1 \dots j_{m+1}} \mathrm{Tr}\left\{\rho X_i^{j_1} X_{i+1}^{j_2} \dots X_{i+m}^{j_{m+1}}\right\} \cdot |j_1 \dots j_{m+1}\rangle = 0 \tag{51}$$

for some i. Then, as the tensor $X_i \dots X_{i+m-1}$ is injective,

$$X_{i+m}^{j_{m+1}} \rho = 0 \quad \forall j_{m+1} \in \{1, 2, \dots, d_{i+m}\}. \tag{52}$$

Take any matrix $M \in \mathbb{C}^{D_i} \otimes \mathbb{C}^{D_{i+1}}$. Then

$$0 = X_{i+1}^{j_2} \dots X_{i+m}^{j_{m+1}} \rho M \in \mathbb{C}^{D_{i+1}} \otimes \mathbb{C}^{D_{i+1}}. \tag{53}$$

Then

$$\sum_{j_2\dots j_{m+1}} \mathrm{Tr}\left\{X_{i+1}^{j_2}\dots X_{i+m}^{j_{m+1}}\rho M\right\}\cdot|j_1\dots j_{m+1}\rangle = 0\ . \tag{54}$$

The block of the m consecutive tensors $X_{i+1}\dots X_{i+m}$ is injective, therefore $\rho M = 0$. As M was arbitrary, $\rho = 0$, thus the MPS is injective after blocking $m+1$ sites. □

Finally, we introduce Matrix Product Operators (MPO).

Definition 6. A *Matrix Product Operator* is an operator written in MPS form:

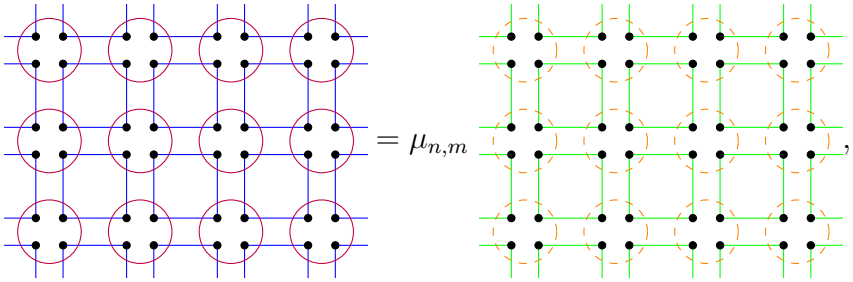
$$V_n(X) = \sum_{i_1\dots i_n, j_1\dots j_n} \mathrm{Tr}\{X^{i_1 j_1}\dots X^{i_n j_n}\}|i_1\dots i_n\rangle\langle j_1\dots j_n|\ . \tag{55}$$

As MPOs are just special MPSs, all the definitions and structure theorems above apply. In particular, we will use the terminology *normal, injective, periodic* for MPOs too.

VI. CANONICAL FORM

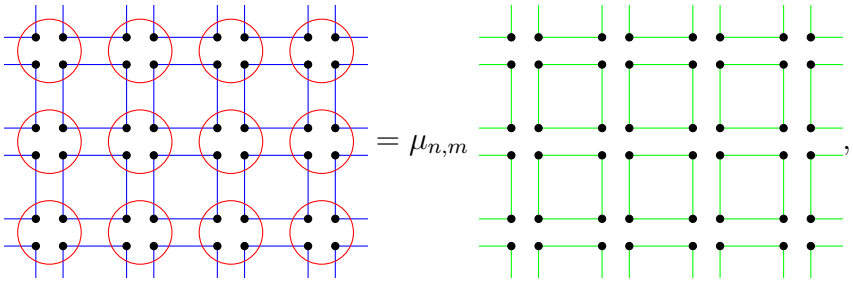
In this section we investigate when two quasi-injective PEPS defined by (ϕ_A, O_A) and (ϕ_B, O_B) describe the same state for some (sufficiently large) system size. We find that this question can be decided locally: the two states are proportional for a large system size if and only if they are proportional on a 3×3 torus. Moreover, the boundary degree of freedoms are related by an invertible MPO whose inverse is also an MPO. Finally, we show that $O_B^{-1}O_A$ has to be a product of two-particle invertible operators. In Appendix A, we also provide some examples that explain why the situation is more complicated than in the case of injective PEPS.

Consider two quasi-injective PEPS generated by (ϕ_A, O_A) and (ϕ_B, O_B). Suppose that on an $n\times m$ torus, they generate states that are proportional to each other:



(56)

where the purple circle and the blue rectangle depicts O_A and $|\phi_A\rangle$, while the orange dashed circle and the green rectangle depicts O_B and $|\phi_B\rangle$ and $\mu_{n,m} \in \mathbb{C}$. Inverting O_B, we obtain



(57)

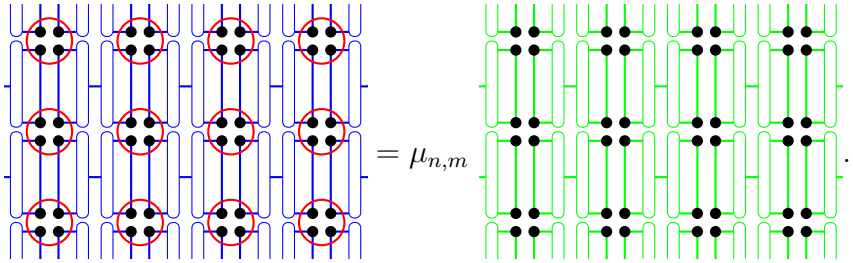
where the red circle denotes the invertible operator $O = O_B^{-1} O_A$. This equation is the starting point of our investigation below. First we prove that it hold for all system sizes:

Proposition 12. *If Eq.* (57) *holds for some* $n_0 \geq 3, m_0 \geq 3$*, then it also holds for any* $n, m \in \mathbb{N}$ *and the proportionality constant is* $\mu_{n,m} = \mu^{nm}$*.*

Proof. Take a minimal rank decomposition of the four-partite states w.r.t. the vertical cut. That is, write

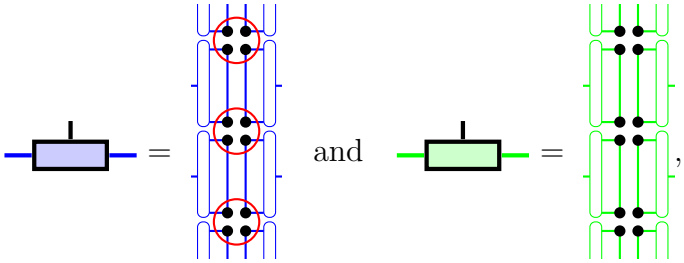
(58)

Using this decomposition, Eq. (57) reads as



(59)

This gives rise to an MPS description of the states with the following tensors:



(60)

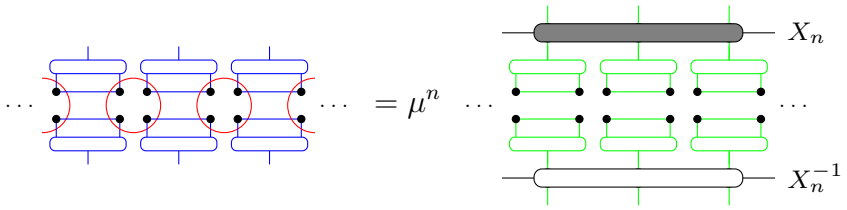
where the physical index of the MPS tensor is all physical indices of the virtual particles, while the virtual indices of the MPS corrspond to the virtual indices of the minimal rank decomposition of the four-partite states. These tensors are injective: the green tensor is just a tensor product of the Schmidt vectors, and as the Schmidt vectors (and their tensor

product) are linearly independent, that tensor is injective. The blue tensor is obtained by acting with an invertible operator on the tensor product of Schmidt vectors, therefore it is also injective.

Thus, using Proposition 7, if Eq. (57) holds for $n_0 \geq 3$, $m_0 \geq 3$, then it also holds when the system size in the horizontal direction is changed to any n by keeping the system size in the vertical direction m_0. Therefore Eq. (57) holds for m_0 and any n, and the proportionality constant is $\mu_{n,m_0} = \mu_{m_0}^n$ for some $\mu_{m_0} \in \mathbb{C}$. The argumentation above holds w.r.t. the horizontal cut. Therefore the system size can be changed along the vertical direction too: as Eq. (57) holds for n, m_0, it also holds for n, m and the proportionality constant is then $\mu_{n,m_0}^{m/m_0} = \mu^{nm}$ for some $\mu \in \mathbb{C}$. □

Note that this implies that it is decidable whether two quasi-injective PEPS are equal for all system size. Moreover, it is also practically checkable: it is enough to calculate the overlap between two states (and their norms) on a 3×3 torus. The overlaps can be calculated by standard tensor network techniques. The cost of this computation scales as the 12th power of the Schmidt rank.

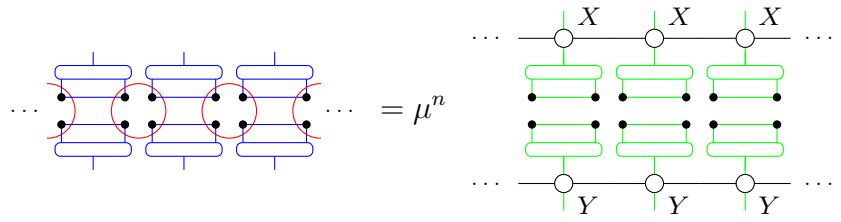
Using Proposition 7, we conclude that up to a constant there is a uniquely defined operator X_n on the boundary for which



(61)

This construction, however, does not reveal anything about the properties of the gauges X_n and X_n^{-1}: they are globally defined and the definition depends on the system size. In the following we explore their structure and show that they can both be written as a normal MPOs.

Theorem 13. *Suppose Eq.* (57) *holds for some* $n, m \geq 3$. *Then there are two MPO tensors* X *and* Y *such that*



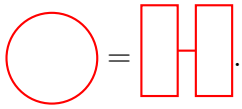
(62)

where $\mu \in \mathbb{C}$ is the proportionality constant from Proposition 12, and $V_n(Y) = (V_n(X))^{-1}$ for every size n and both X and Y become injective after blocking two tensors.

Before proceeding to the proof, notice that

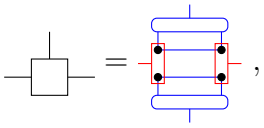
Lemma 14. *The l.h.s. of Eq.* (62) *can be described by an MPS that becomes injective after blocking two tensors.*

Proof. Take a minimal rank decomposition of the operators O:



(63)

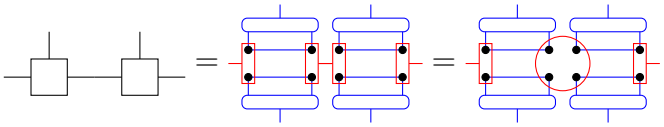
Then the l.h.s. of Eq. (62) is an MPS with MPS tensor



(64)

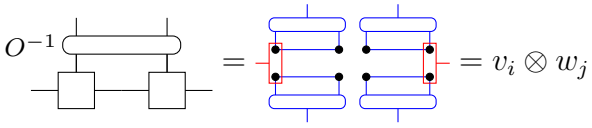
where the physical indices of the MPS are both the physical indices and the two virtual indices belonging to the decomposition of $|\phi_A\rangle$ on the r.h.s. of Eq. (64), while the virtual indices of the MPS are the virtual indices belonging to the decomposition of O on the r.h.s. of Eq. (64).

We prove now that this MPS tensor is injective after blocking two tensors. To see this, block two tensors and note that contracting the middle indices gives back O:



(65)

Inverting O does not change the injectivity of the MPS tensor, as it is an invertible operation on its physical indices. Therefore it is enough to prove that

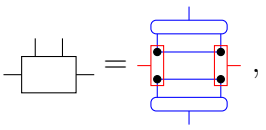


(66)

is injective. Both v_i and w_j are linearly independent, as the Schmidt vectors of O are linearly independent and the one body reduced densities of the four-partite states are full rank. Therefore the vectors $v_i \otimes w_j$ are also linearly independent, that is, the corresponding tensor is injective. □

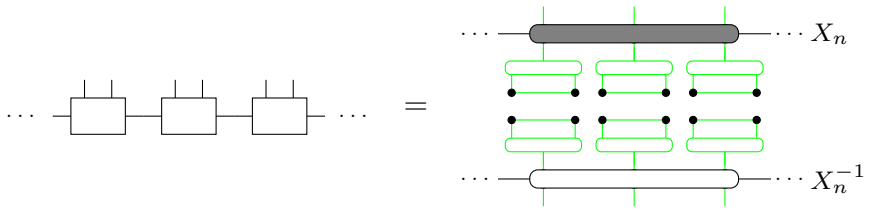
We now proceed to the proof of Theorem 13.

Proof of Theorem 13. We first prove that X_n and X_n^{-1} are proportional to an MPS. Write the l.h.s. of Eq. (61) as an MPS with two physical indices:



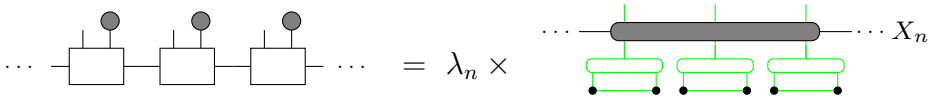
(67)

where the left physical index of the MPS tensor corresponds to the indices on the top of the r.h.s. (physical and virtual indices of the Schmidt vector), while the right one to the indices on the bottom of the r.h.s., and the virtual indices of the MPS correspond to the Schmidt index of the decomposition of O. With this notation, Eq. (61) reads as



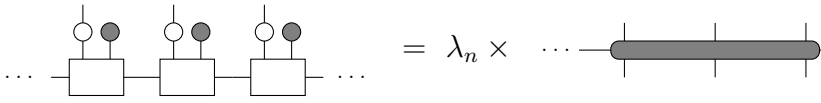
(68)

Applying a product linear functional on the lower half of the r.h.s. (and the right indices of the MPS on the l.h.s.), the equation changes to



(69)

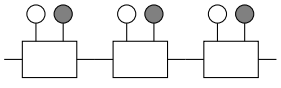
for some $\lambda_n \in \mathbb{C}$. Notice that the Schmidt vectors on the r.h.s. can be inverted: they are an injective mapping from the Schmidt index to the physical degrees of freedom, as they are linearly independent. Therefore,



(70)

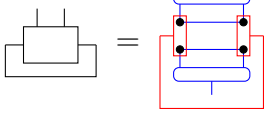
where the white circle depicts the inverse of the Schmidt vectors of $|\phi_B\rangle$. This shows that X_n (and similarly X_n^{-1}) is an MPS with some MPS tensor $\tilde{X}$ (and $\tilde{Y}$) as long as the l.h.s. is not 0. It is thus sufficient to prove that there is a translationally invariant product linear functional (the gray circles), which is independent of n, that does not map the l.h.s. to 0.

Consider two linear functionals acting on the MPS tensor:



(71)

We show now that there are linear functionals a, b such that for the corresponding $M_{a,b}$ $\mathrm{Tr}\{M_{a,b}\} \neq 0$. Let us consider the map $F : (a, b) \mapsto \mathrm{Tr}\{M_{a,b}\}$. Graphically, this map is

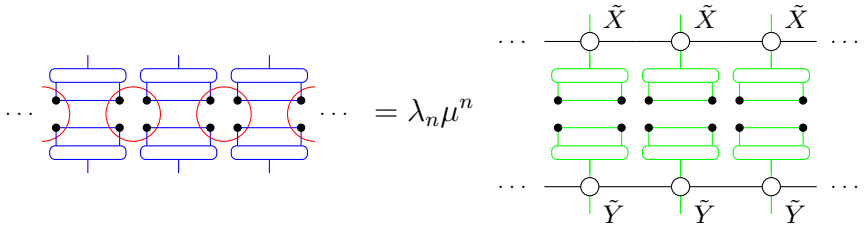
$F =$  . (72)

Notice that F equals to the operator O with left and right side interchanged applied to the tensor product of the Schmidt vectors of $|\phi\rangle$. As O is invertible, F is not zero. Therefore there are linear functionals a, b such that $F(a, b) = \mathrm{Tr}\{M_{a,b}\} \neq 0$. As $\mathrm{Tr}\{M_{a,b}\} \neq 0$, $M_{a,b}$ is not nilpotent and thus

$$\mathrm{Tr}\{M_{a,b}^n\} = \sum_{i=1}^{R} \xi_i^n \tag{73}$$

for some $\xi_1, \ldots \xi_R \in \mathbb{C}\backslash\{0\}$, $R > 0$. Let $S := \{n \in \mathbb{N} \mid \mathrm{Tr}\{M_{a,b}^n\} \neq 0\}$. Notice that $|S| = \infty$. Then, choosing the linear functional appearing in Eq. (70) to be b, the l.h.s. is non-zero for all system sizes $n \in S$. Therefore, X_n can be written as an MPO for all $n \in S$. Similarly, using the linear functional a instead of b on the lower part of Eq. (68), we arrive to the conclusion that X_n^{-1} is also a non-zero MPO for all $n \in S$, for the same S.

Therefore there is a $\lambda_n \in \mathbb{C}$ such that $\forall n \in S$,



. (74)

Here, μ_n is the proportionality constant appearing in Eq. (62), and $V_n(\tilde{X})$ and $V_n(\tilde{Y})$ are translationally invariant MPOs on n sites, such that $V_n(\tilde{Y}) = \left(V_n(\tilde{X})\right)^{-1}/\lambda_n$. Their defining tensors, $\tilde{X}$ and $\tilde{Y}$ are independent of n. Note that the MPOs $V_n(\tilde{X})$ and $V_n(\tilde{Y})$ are defined for $\forall n \in \mathbb{N}$, but we have not yet proven that Eq. (74) holds for $n \notin S$.

In the following we prove that Eq. (74) also holds $\forall n \in \mathbb{N}$ for some injective MPO $V_n(X)$, $V_n(Y)$ with $\lambda_n = 1$.

Using Corollary 9.1, there exists $K \in \mathbb{N}$ such that after blocking K tensors, both $V_n(\tilde{X})$ and $V_n(\tilde{Y})$ ($n \in K\mathbb{N}$) can be decomposed into a linear combination of normal MPOs. As the tensor product of normal MPSs is again a normal MPS (Proposition 6), $V_n(\tilde{X}) \otimes V_n(\tilde{Y})$ has a decomposition into normal MPO that are tensor products. Denote these essentially

different normal MPO by $V_n(X_i) \otimes V_n(Y_i)$. That is, $\forall n \in K\mathbb{N}$

$$V_n(\tilde{X}) \otimes V_n(\tilde{Y}) = \sum_{i=1}^{L} \sum_{j=1}^{M_i} \zeta_{ij}^n V_n(X_i) \otimes V_n(Y_i), \tag{75}$$

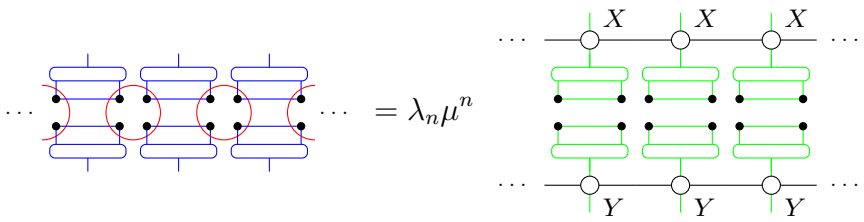
where $V_n(X_i) \otimes V_n(Y_i)$ are essentially different normal MPOs. Using this decomposition in Eq. (74), the l.h.s. is described by a normal MPO (Lemma 14), while the r.h.s. is described by the sum above for an infinite number of system sizes (indeed, for all $n \in K\mathbb{N} \cap S$). As essentially different MPSs become linearly independent for large system sizes (Corollary 7.1), Eq. (75) can describe a normal MPO only if either $L = 1$ or otherwise all but one i satisfy

$$\sum_{j=1}^{M_i} \zeta_{ij}^n = 0 \quad \forall n \in S \cap K\mathbb{N}. \tag{76}$$

Recalling that Eq. (73) vanishes $\forall n \in \mathbb{N} \backslash S$, we conclude that

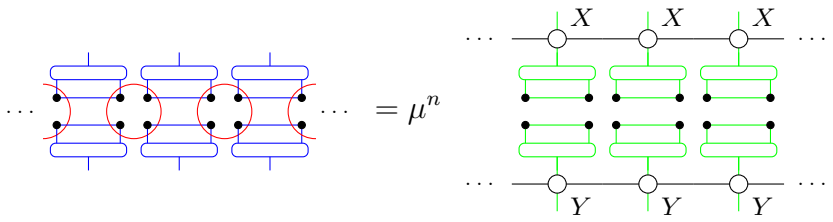
$$\sum_{k=1}^{R} \xi_k^n \sum_{j=1}^{M_i} \zeta_{ij}^n = \sum_{kj} (\xi_k \zeta_{ij})^n = 0 \quad \forall n \in K\mathbb{N}, \tag{77}$$

where i is chosen such that the sum of ζ_{ij}^n vanishes $\forall n \in S \cap k\mathbb{N}$. Applying Proposition 10 to Eq. (77), all $(\xi_k \zeta_{ij})^K = 0$, that is, $\zeta_{ij} = 0$ for all j and all but one i. Therefore, $L = 1$ in Eq. (75). Using Proposition 9, we conclude that $V_n(\tilde{X}) \otimes V_n(\tilde{Y})$ does not contain periodic MPO, therefore $K = 1$. Thus, both the l.h.s. and the r.h.s. of Eq. (74) are proportional to normal MPOs. Using Proposition 7, we conclude that the equality in Eq. (74) holds $\forall n \in \mathbb{N}$. We have therefore proven that there are normal MPO tensors X and Y (the ones appearing in the unique normal MPO in Eq. (75)) such that $\forall n \in \mathbb{N}$ and some $\lambda_n \in \mathbb{C}$



(78)

These MPO tensors also satisfy $V_n(Y) = (V_n(X))^{-1} / \lambda_n$ for all $n \in S$. As both $V_n(Y)$ and $V_n(X)$ are normal MPOs, the equality holds $\forall n \in \mathbb{N}$ and thus $\lambda_n = \lambda^n$ for some $\lambda \in \mathbb{C}$. Absorbing this constant into Y, $V_n(Y) = (V_n(X))^{-1}$ and



(79)

□

Corollary 14.1. *Suppose that* $\forall n \in \mathbb{N}$ *Eq.* (62) *holds also for some other MPO* $V_n(\tilde{X})$ *and* $V_n(\tilde{Y})$ *and* $V_n(\tilde{Y}) = \left(V_n(\tilde{X})\right)^{-1}$. *Then* $V_n(\tilde{X}) = \lambda^n V_n(X)$ *and* $V_n(\tilde{Y}) = \lambda^{-n} Y^{(n)}$ *for some* $\lambda \in \mathbb{C}$.

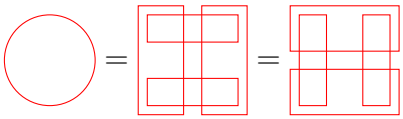
Proof. Due to uniqueness of the gauge in Eq. (61), $V_n(\tilde{X}) = \lambda_n V_n(X)$ and $V_n(\tilde{Y}) = \lambda_n^{-1} V_n(Y)$. Decomposing $V_n(\tilde{X})$ and $V_n(\tilde{Y})$ to their canonical forms, we see that the only normal MPS appearing in the decomposition is $V_n(X)$ and $V_n(Y)$, and that $\lambda_n = \sum_i \lambda_i^n$ and $\lambda_n^{-1} = \sum_i \eta_i^n$. But then $1 = \sum_{ij} (\lambda_i \eta_j)^n$ and thus by Proposition 10, $\lambda_n = \lambda^n$. □

It turns out that the fact that the boundaries of the two quasi-injective PEPS are related by an MPO severely restricts the form of O. We will indeed find that

Proposition 15. *The operator* O *from Eq.* (57) *can be written as a product of invertible two-body operators:*

$$O = (O_{14} \otimes O_{23}) \cdot (O_{12} \otimes O_{34}) = \left(\tilde{O}_{12} \otimes \tilde{O}_{34}\right) \cdot \left(\tilde{O}_{14} \otimes \tilde{O}_{23}\right) \ , \tag{80}$$

where the particles are numbered clockwise from the upper left corner and O_{ij} *acts on particles* i *and* j. *Pictorially,*



(81)

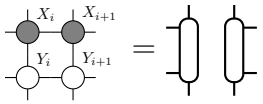
We will prove that O has a four site long non-translationally invariant MPO decomposition, with the property that cutting the MPO into two halves yields a minimal rank decomposition of O. Moreover, we will show that the product of the Schmidt vectors of O and O^{-1} are tensor products. Before proceeding to the proof, we show that if O and O^{-1} are both MPO of this form, O has to have the two-layer structure (81).

Lemma 16. *Consider two non-translationally invariant MPOs on* $n = 2k$ *sites with tensors* $X_1, \ldots X_n$ *and* $Y_1, \ldots Y_n$. *Suppose that*

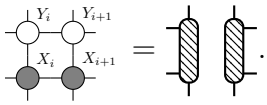
1. $V(X_1, \ldots, X_n) \cdot V(Y_1, \ldots, Y_n) = \mathrm{Id}$

2. *Both* $X_i X_{i+1}$ *and* $Y_i Y_{i+1}$ *are injective for all* $i = 1, \ldots, n$ *with* $n + 1 \equiv 1$.

3. The product of X_iX_{i+1} and Y_iY_{i+1} factorizes as depicted:

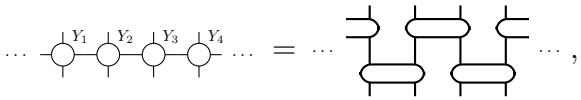


(82)



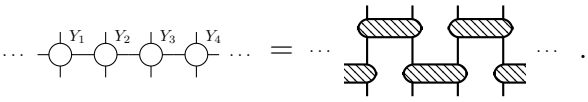
(83)

Then $V(X_1, \ldots, X_n)$ (and $V(Y_1, \ldots, Y_n)$) admits a two layer description:



(84)

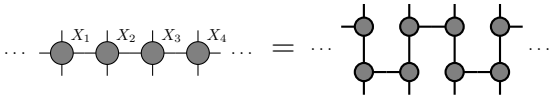
where all two-body operators on the r.h.s. are invertible. Eq. (84) *also holds when shifted by one site (with other invertible operators):*



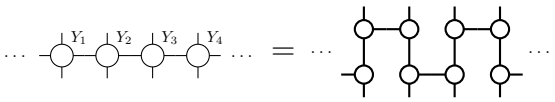
(85)

Note that for the translationally invariant setting, conditions 2 and 3 are satisfied naturally after blocking some tensors.

Proof. Take a Schmidt decomposition of the tensors $X_1, \ldots, X_n$ and $Y_1, \ldots, Y_n$ in an alternating way:

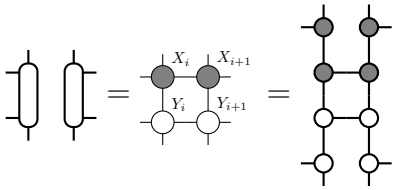


(86)



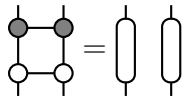
(87)

We will prove that the two-body operators defined this way are invertible. They naturally have to be injective from the outside to the middle indices, otherwise $V(X_1, \ldots X_n)$ and $V(Y_1, \ldots Y_n)$ would not be invertible. Suppose that there is an operator which is not injective from the middle to the outside. Suppose it happens in the lower layer of $V(X_1, \ldots X_n)$. Consider a 2-site part of the MPO.



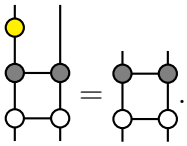
(88)

As we took a minimal rank decomposition, the outer tensors on the l.h.s. are invertible. Therefore, the product of the operators in the middle is a product:



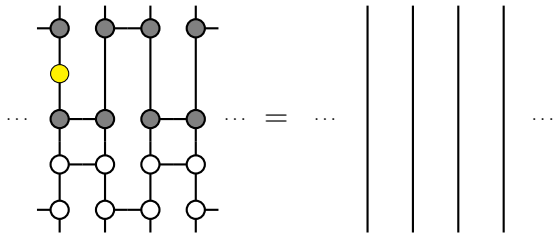
(89)

Therefore if the gray operator is not injective from top to bottom, then its kernel factorizes. Suppose the left operator on the r.h.s. has a non trivial kernel. Then we can insert a non-trivial projector y on top that does not change the value of the product:



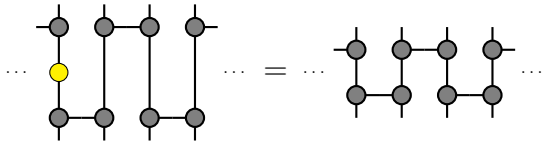
(90)

Inserting this back into the product $V(X_1, \dots X_n) \cdot V(Y_1, \dots Y_n)$, we get that



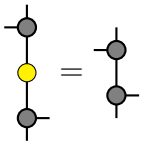
(91)

As $V(Y_1, \dots Y_n)$ is invertible, its left inverse is unique and equal to $V(X_1, \dots, X_n)$. Therefore



(92)

By assumption, the tensors defining the MPO are injective after blocking at least two sites. Therefore, by inverting all but one tensor, we conclude that

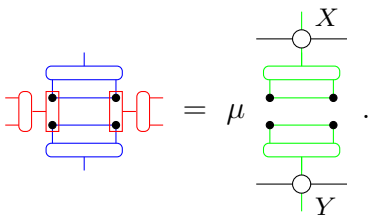


(93)

But this is not possible unless the yellow tensor is the identity. Thus, the two-body operators are invertible. □

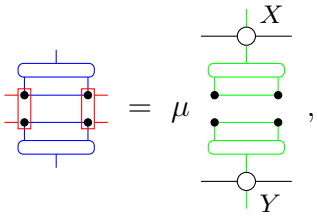
We now proceed to the proof of Proposition 15. Note that it is enough to show that both O and O^{-1} admit an MPO description that satisfy the conditions of Lemma 16.

Proof of Proposition 15. Write the l.h.s. of Eq. (62) as an injective MPS with tensors defined in Eq. (64). The r.h.s. of Eq. (62) is also an injective MPS. Therefore, the generating tensors are related by a gauge transformation:



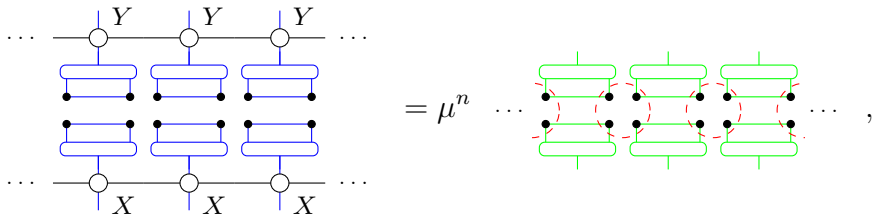
(94)

Absorbing the gauge in the decomposition of the operator, we have



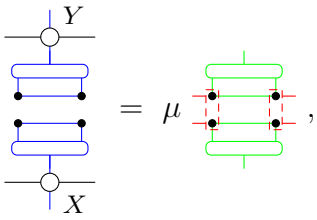
(95)

where the red rectangles depict a minimal rank decomposition of the operator O. As $V_n(X)$ and $V_n(Y)$ are inverses of each other, the inverse relation of Eq. (62) reads



(96)

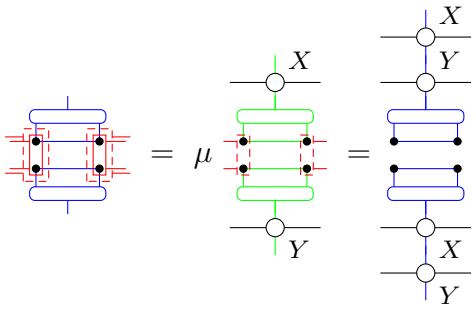
where the dashed red circles denote O^{-1}. Therefore, with an appropriate minimal rank decomposition of O^{-1}, the generating tensors are related as follows:



(97)

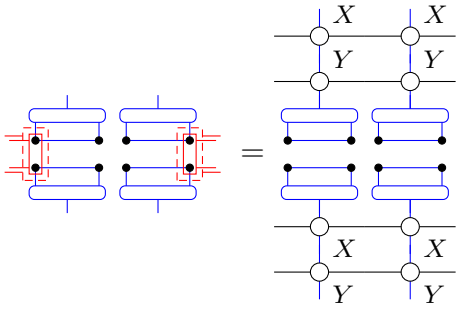
where the dashed rectangles denote the Schmidt decomposition of O^{-1}. Therefore, applying

the Schmidt vectors of O and then O^{-1} to the Schmidt vectors of $|\phi_A\rangle$, we obtain



(98)

Contracting two copies of Eq. (98), the middle operator is $OO^{-1} = \mathrm{Id}$, so

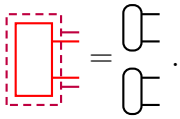


(99)

Notice that the l.h.s. is a product w.r.t. the vertical cut, whereas the r.h.s. is product w.r.t. the horizontal cut. Therefore both sides have to be product w.r.t. both vertical and horizontal cuts. Note that then $V_n(X)$ and $V_n(Y)$ satisfy the conditions of Lemma 16 and thus are products of invertible two-body operators in the sense of Eqs. (84) and (85). Similarly, both terms on the l.h.s. factorize w.r.t. the horizontal cut. As the one-body reduced densities of $|\phi_A\rangle$ are full rank, the product of the Schmidt vectors of O and O^{-1} factorize:

$$\left(O^{-1}\right)^{(13)}_{kl} O^{(13)}_{ij} = A^{(1)}_{ik} \otimes A^{(3)}_{jl}. \tag{100}$$

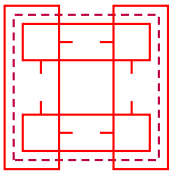
The same holds for the Schmidt vectors of all neighboring bipartition in any order. Similarly, the equation holds for the bipartition $(13) - (24)$ and also for the reordering of O and O^{-1}. Eq. (100) can be pictorially represented as



(101)

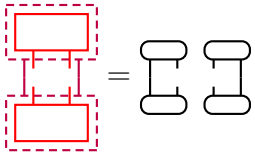
Consider the operator

$$Z = \left(O^{(13)}_{j_1 j_2} \otimes O^{(24)}_{j_3 j_4}\right) O^{-1} \left(O^{(12)}_{i_1 i_2} \otimes O^{(34)}_{i_3 i_4}\right) = \tag{102}$$



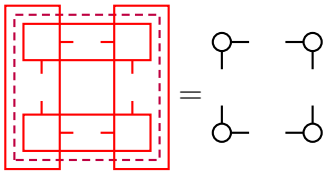
Note that Z factorizes w.r.t. the bipartition $(13)-(24)$: to see this, decompose O^{-1} w.r.t. the bipartition $(12)-(34)$. Then

$$O^{-1}\left(O^{(12)}_{i_1 i_2} \otimes O^{(34)}_{i_3 i_4}\right) = \tag{103}$$



therefore it factorizes w.r.t. the bipartition $(13)-(24)$, and so does Z. Similarly, Z also factorizes w.r.t. the bipartition $(12)-(34)$. Therefore, Z is a four-partite product,

$$Z = \tag{104}$$



As contracting the open indices of Z gives back the operator $OO^{-1}O = O$, and as Z has a tensor product structure, this construction gives rise to an MPO description of O. Similarly, contracting only the vertical (horizontal) indices the lower (upper) two layers gives $O^{-1}O = \mathrm{Id}$ ($OO^{-1} = \mathrm{Id}$) on the lower (upper) two layers, and thus we obtain a minimal rank decomposition of O in the horizontal (vertical) cut. As the Schmidt vectors are linearly independent, the MPO tensors become injective after blocking two tensors.

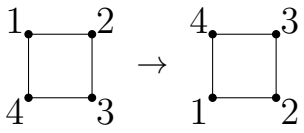
The above construction can be repeated for O^{-1}. This leads to an MPO decomposition of O^{-1}.

These two decompositions satisfy the conditions of Lemma 16: the MPOs become injective after blocking two tensors, moreover, the product of two neighboring tensors of O and O^{-1} factorizes. Therefore, O (and O^{-1}) is a product of invertible two-body operators. □

The above form provides an equivalent characterization of when two quasi-injective PEPS are equal for all system sizes. Before stating the theorem, we introduce two swap operators on four particles. The horizontal swap, H_A, exchanges the virtual particles of $|\phi_A\rangle$ in the horizontal direction:

$$\begin{array}{cc} 1 & 2 \\ 4 & 3 \end{array} \rightarrow \begin{array}{cc} 2 & 1 \\ 3 & 4 \end{array} . \tag{105}$$

The vertical swap, V_A, reflects the particles of $|\phi_A\rangle$ in the vertical direction:

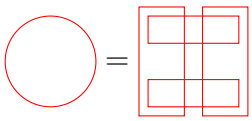


(106)

We denote the product of H_A and V_A as S_A: $S_A = H_A V_A = V_A H_A$. Define H_B, V_B and S_B similarly for $|\phi_B\rangle$. Note that H_A and H_B are different in general as the Hilbert spaces of the virtual particles might differ.

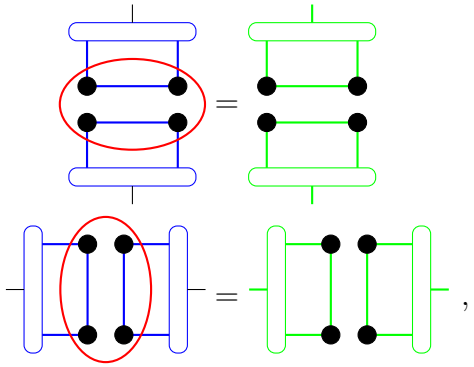
Theorem 17. *Two quasi-injective PEPS are equal (Eq.* (57) *holds) if and only if the following conditions are satisfied:*

- *The operator O factorizes into two-body operators as*



(107)

- *The Schmidt vectors of the four-partite states satisfy:*



(108)

(109)

where the horizontal ellipse denotes $H_B O H_A$, and the vertical ellipse denotes $V_B O V_A$.

Note that the last two conditions are equivalent to the property that the two states are equal on an $n \times 1$ and a $1 \times n$ torus for all n, therefore they are easily checkable.

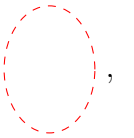
Proof. The necessity of these conditions is clear from above. We now prove the sufficiency.

Let

$$O^{-1} = \quad , \tag{110}$$

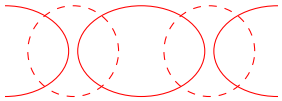
$$H_B O H_A = \quad , \tag{111}$$

$$V_A O^{-1} V_B = \quad , \tag{112}$$



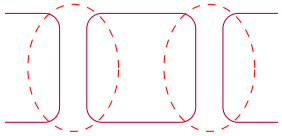
$$S_B O S_A = \quad . \tag{113}$$

Due to the two layer structure of O and O^{-1} (Eq. (81)), the following operator is a product in the horizontal cut:



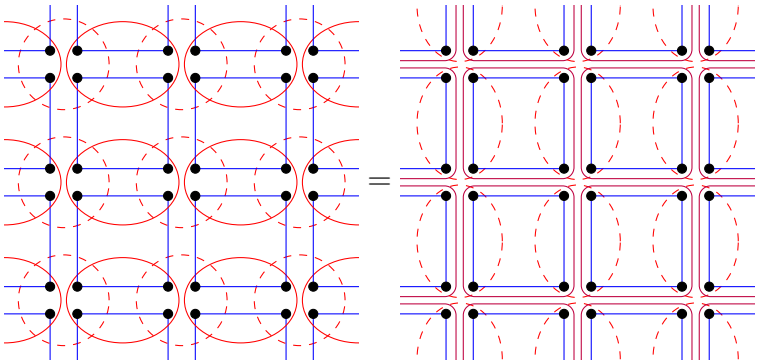
$$= A \otimes B \ , \tag{114}$$

where $H_B O H_A$ is the lower layer. The vertical swap of the previous operator is



$$= B \otimes A \ , \tag{115}$$

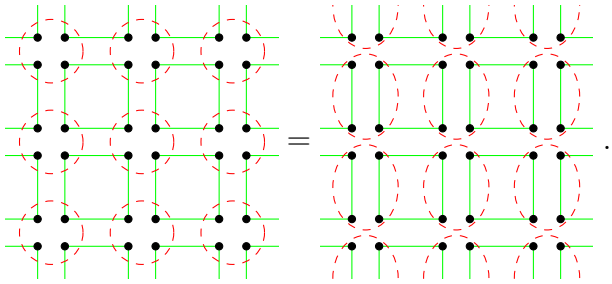
where $S_B O S_A$ is the lower layer. Consider now these operators acting on the quasi-injective PEPS defined by $|\phi_A\rangle$ and Id:



$$= \tag{116}$$

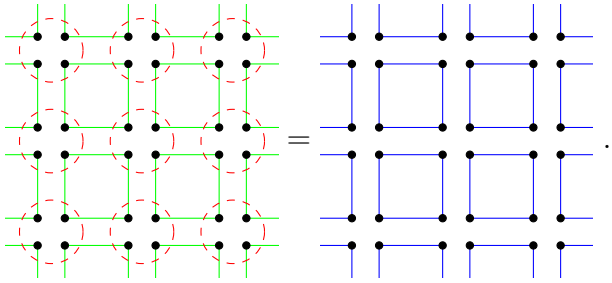
From Eq. (108) and (109), the action of the lower layers on each side is to change $|\phi_A\rangle$ to

$|\phi_B\rangle$. Therefore,



(117)

Using once more Eq. (109), the r.h.s. is a tensor product of ϕ_A at every position:



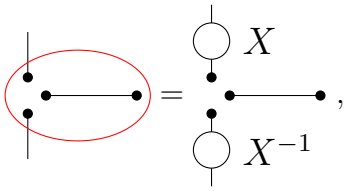
(118)

applying O on both sides on each site, we see that Eq. (57) holds. □

As a simple application, one can derive the canonical form of injective PEPS[35].

Corollary 17.1. *Two injective PEPS generate the same state if and only if they are related by a product gauge transformation.*

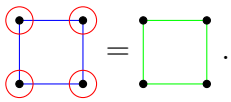
Proof. The conditions of Theorem 17 that Schmidt vectors map to Schmidt vectors read as



(119)

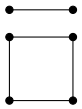
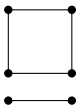
therefore the operator O is a product on the two leftmost particles (and on one particle it is the inverse of the other). Similarly the other condition implies that the operator is a product on the two rightmost particles. Therefore O has a product structure in the desired form. □

We now show that if the span of the Schmidt vectors of both states w.r.t. both the vertical and horizontal cut contain product states, then $|\phi_A\rangle$ and $|\phi_B\rangle$ are SLOCC[47]-equivalent, that is, there are invertible operators O_1, O_2, O_3, O_4 acting on the virtual particles such that $O_1 \otimes O_2 \otimes O_3 \otimes O_4 |\phi_A\rangle = |\phi_B\rangle$. Pictorially,



(120)

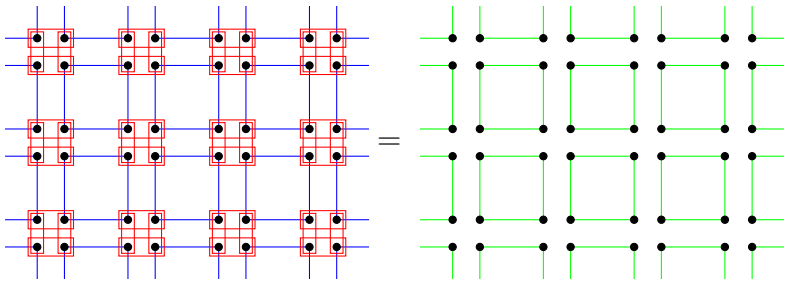
Note that there are examples for states that don't have product states in the span of their Schmidt vectors, but they generate the same state and are not SLOCC equivalent. For example consider

$|\phi_A\rangle =$  , $\quad |\phi_B\rangle =$  , (121)

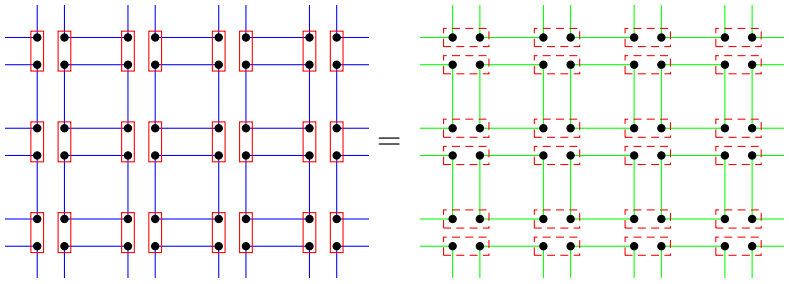
then the quasi-injective PEPS defined by $|\phi_A\rangle$ and Id and $|\phi_B\rangle$ and Id (more precisely the isomorphism that rearranges the tensor product to the right order) are the same on every torus, yet these states are not SLOCC equivalent.

Theorem 18. *If the span of the Schmidt vectors of both four-partite states in Eq.* (57) *contains a product state for both the vertical and horizontal cut on both sides, then the two four-partite states are SLOCC equivalent.*

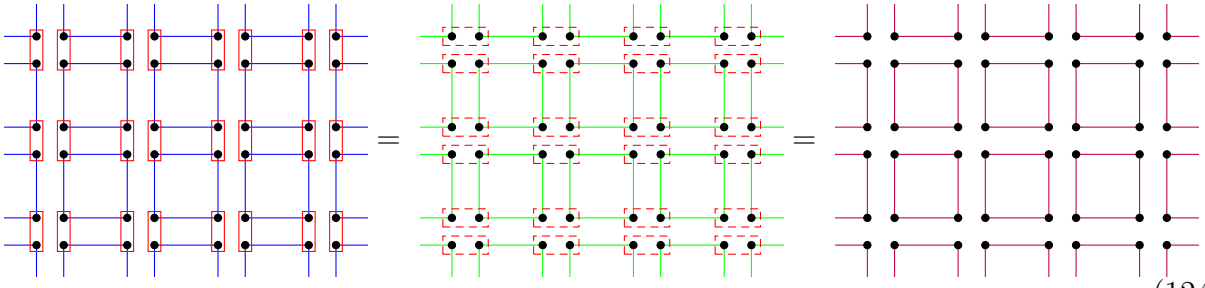
Proof. By Theorem 17, Eq. (57) implies

 (122)

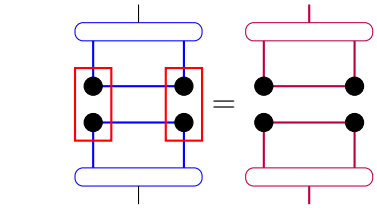
Inverting the upper layer, we get

 (123)

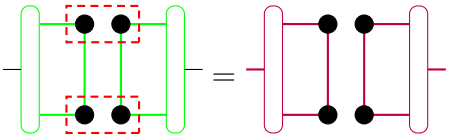
The l.h.s. is product in the vertical direction, the r.h.s. in the horizontal direction. Therefore the two sides describe a state that factorizes in both directions. Let $|\xi\rangle$ be this state and denote this state with a purple square. Then,

 (124)

Equivalently, for the Schmidt vectors we get

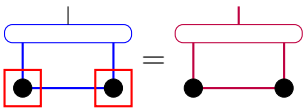


(125)



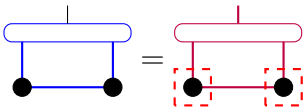
(126)

If the span of the Schmidt vectors on the l.h.s. contains a product vector, the same is true for the Schmidt vectors on the r.h.s. Therefore, choosing a product Schmidt vector on the bottom in Eq. (125) and applying a product linear functional, we get that for some not necessarily invertible operators,



(127)

A similar equation also holds for the lower part, as well as for both sides of $|\phi_B\rangle$. Inverting the operators appearing in Eq. (125), by the same argument, we obtain the inverse relation



(128)

and similarly along all other cuts. Eq. (127) and (128) ensure that the one particle operators can be chosen invertible, thus $|\phi_A\rangle$ and $|\xi\rangle$ are SLOCC equivalent. Similarly, $|\phi_B\rangle$ and $|\xi\rangle$ are SLOCC equivalent. Therefore $|\phi_A\rangle$ and $|\phi_B\rangle$ are SLOCC equivalent. □

Corollary 18.1. *If two quasi-injective PEPS, defined by qubit four-partite states with genuine four-partite entanglement, are equal, then the four-partite states are SLOCC equivalent.*

Proof. Notice that if the four-partite states are entangled for both the vertical and horizontal cut, then the span of the Schmidt vectors is at least two-dimensional. As any two-dimensional subspace contains a product vector, the previous theorem applies. □

Based on Corollary 18.1, we provide a full classification of quasi-injective PEPS defined with four-partite qubit states in Appendix C.

VII. SPT PHASES

In this section we show how the third cohomology labeling of the SPT phases[38,48] extends to quasi-injective PEPS. First, we show how to assign an element from the third cohomology group $H^3(G, \mathbb{C}^*)$ to a (projective) MPO representation of G. Here, and in the following, the action of G on $\mathbb{C}^*$ is trivial. Second, given a group of on-site symmetries of an quasi-injective PEPS, there are three MPO representations associated to it: the boundary along the vertical cut, the boundary along the horizontal cut and finally the symmetry operators themselves. We show that the associated third cohomology labels coincide. The importance of this statement is twofold. First, the labeling is encoded in the local operators already, thus one does not have to look at the boundary of the system to find the labeling. Second, the labeling corresponding the vertical and horizontal boundary coincides despite the model not necessarily having rotational symmetry.

A. Third cohomology labeling of MPO representations

Consider a group G and a projective MPO representation thereof, that is, a tensor X_g that generates an MPO $V_n(X_g)$ for all $g \in G$ such that $V_n(X_g)V_n(X_h) = \lambda_n(g,h)V_n(X_{gh})$ for all $g, h \in G$, where $\lambda_n(g,h) \in \mathbb{C}$. We will restrict ourselves to MPO representations for which $\lambda_n(g,h) = \lambda^n(g,h)$. We call such MPO projective representations *one-block projective MPO representations*. In this section, we show how to assign an element from the third cohomology group $H^3(G, \mathbb{C}^*)$ to such a representation.

We first show that we can suppose w.l.o.g. that X_g is normal. The proof is analogous to Theorem 13.

Lemma 19. *Let $g \mapsto \tilde{X}_g$ be a one-block projective MPO representation of a group G, that is, $V_n(\tilde{X}_g)V_n(\tilde{X}_h) = \lambda^n(g,h)V_n(\tilde{X}_{gh})$ for some $\lambda(g,h) \in \mathbb{C}$. Then $\forall g \in G$ there is a normal tensor X_g such that $V_n(\tilde{X}_g) = V_n(X_g)$.*

Proof. First we prove that $V_n(\tilde{X}_e) = \mu^n \mathrm{Id}$ for some $\mu \in \mathbb{C}$, therefore there is a normal tensor X_e such that $V_n(\tilde{X}_e) = V_n(X_e)$. Then, as $V_n(\tilde{X}_g)V_n(\tilde{X}_{g^{-1}}) = \lambda^n(g, g^{-1})\mu^n \mathrm{Id}$, we will see that $V_n(\tilde{X}_g)$ can also be described with a normal MPO.

To see that $V_n(\tilde{X}_e) = \mu^n \mathrm{Id}$, notice that, as $g \mapsto V_n(\tilde{X}_e)$ is a representation, $V_n(\tilde{X}_e) = \mu_n \mathrm{Id}$ and that $V_n(\tilde{X}_e)V_n(\tilde{X}_e) = \mu_n^2 \mathrm{Id} = \mu_n \lambda^n(e,e)\mathrm{Id}$. Therefore, $\mu_n = \lambda^n(e,e)$.

Let K be such that after blocking K tensors, $V_n(\tilde{X}_g)$ and $V_n(\tilde{X}_{g^{-1}})$ can be decomposed into a sum of N and M normal MPOs, respectively. That is, $\forall n \in K\mathbb{N}$

$$V_n(\tilde{X}_g) = \sum_{i=1}^{N} V_n(\tilde{X}_g^{(i)}), \tag{129}$$

$$V_n(\tilde{X}_{g^{-1}}) = \sum_{i=1}^{M} V_n(\tilde{X}_{g^{-1}}^{(i)}). \tag{130}$$

Then their product, $\lambda^n(g, g^{-1})\mu^n \mathrm{Id}$, can be decomposed into a sum of at least MN not necessarily essentially different normal MPOs:

$$\lambda^n(g, g^{-1})\mu^n \mathrm{Id} = \sum_{i=1}^{N}\sum_{j=1}^{M} V_n(\tilde{X}_g^{(i)}) V_n(\tilde{X}_{g^{-1}}^{(j)}). \tag{131}$$

Let L be such that after blocking L tensors, all of these MPOs can be decomposed into normal MPOs: $\forall n \in KL\mathbb{N}$

$$\lambda^n(g, g^{-1})\mu^n \mathrm{Id} = \sum_{i=1}^{N}\sum_{j=1}^{M}\sum_{k=1}^{K_{ij}} V_n(Z_g^{ijk}), \tag{132}$$

for some normal tensors Z_g^{ijk}. If $i \neq i'$ or $j \neq j'$, Z_g^{ijk} and $Z_g^{i'j'k'}$ are not necessarily essentially different. Collecting the essentially different terms yields

$$\lambda^n(g, g^{-1})\mu^n \mathrm{Id} = \sum_{i=1}^{R}\sum_{j=1}^{S_i} \xi_j^n V_n(Z_g^i), \tag{133}$$

where R is the number of essentially different terms, Z_g^i are a maximal pairwise essentially different subset of Z_g^{ijk} and S_i is the multiplicity with which Z_g^i appears. Note that

$$\sum_{i=1}^{R} S_i = \sum_{i=1}^{N}\sum_{j=1}^{M} K_{ij}. \tag{134}$$

As essentially different normal MPOs become linearly independent for sufficiently large system sizes (Corollary 7.1), Proposition 10 implies that there can only be one term in this decomposition, that is, $R = 1$ and moreover $S_1 = 1$. As all $K_{ij} \geq 1$, we have $N = M = 1$ and thus $V_n(\tilde{X}_g)$ is normal. Therefore, $V_n(\tilde{X}_g)$ can be described by a normal MPO tensor X_g. □

The central tool in this section is comparing normal and non-normal MPS tensors that generate the same state. We only state the results here, the proofs are provided in Appendix B.

Proposition 20. *Let A be a normal MPS tensor, B an MPS tensor such that for some $\lambda \in \mathbb{C}$*

$$V_n(B) = \lambda^n V_n(A) \quad \forall n \in \mathbb{N}. \tag{135}$$

Then there exist matrices V, W such that $VW = \mathrm{Id}$ and $\forall n \in \mathbb{N}$ and $(i_1, i_2 \dots i_n) \in \{1, 2, \dots d\}^n$,

$$V B^{i_1} \dots B^{i_n} W = A^{i_1} \dots A^{i_n} \tag{136}$$

Definition 7. The pair of operators V, W in Proposition 20 is called a *reduction* from B to A.

Proposition 21. *Let V, W be a reduction from B to A. Let $N^i = B^i - W A^i V$. Then the algebra generated by N^i is nilpotent.*

Definition 8. Let V, W be a reduction from B to A. Let $N^i = B^i - W A^i V$. Then the *nilpotency length* of the reduction is the minimal N_0 such that $\forall n \geq N_0$

$$N^{i_1} \dots N^{i_n} = 0. \tag{137}$$

The main statement is that any two reductions are related:

Theorem 22. *Let V, W and $\tilde{V}, \tilde{W}$ be two reductions from B to a normal tensor A. Let the nilpotency length of both reductions be at most N_0. Then $\exists \lambda \in \mathbb{C}$ such that for any $n > 2N_0$,*

$$V B^{i_1} B^{i_2} \dots B^{i_n} = \lambda \tilde{V} B^{i_1} B^{i_2} \dots B^{i_n} \tag{138}$$

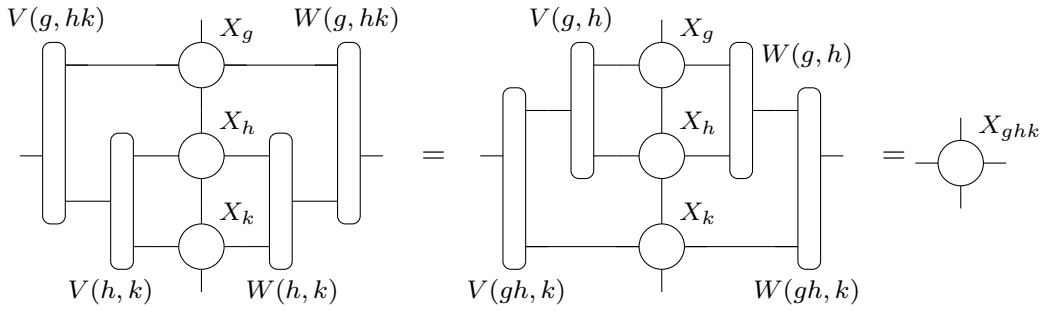
$$B^{i_1} B^{i_2} \dots B^{i_n} W = \lambda^{-1} B^{i_1} B^{i_2} \dots B^{i_n} \tilde{W}. \tag{139}$$

Let us now continue how to assign an element of the third cohomology group to a one-block projective MPO representation. This discussion is essentially the same as in Ref. 38. We include here the construction for completeness.

Let $X_{g,h} = \sum_{ijk} X_g^{ij} \otimes X_h^{jk} \otimes |i\rangle\langle k|$ be the MPO tensor describing the product of two MPOs. As $X_{g,h}$ and X_{gh} describe the same state and X_{gh} is injective, $X_{g,h}$ can be reduced to X_{gh} by Proposition 20. Let us fix such a reduction $V(g,h), W(g,h)$ for any pair of group elements. We will assign a complex scalar to these reductions. We show that this scalar forms a three-cocycle. Different reductions then lead to different three-cocycles. We show,

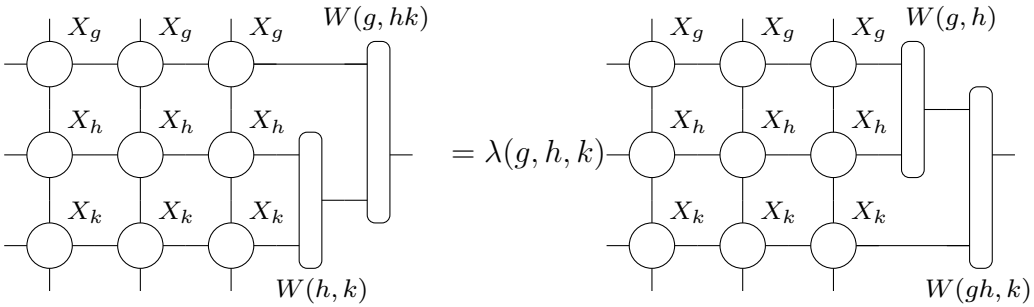
however, that their ratio forms a three-coboundary. Therefore, the equivalence class of the scalars is an element from the third cohomology group.

Starting from the reductions $V(g,h)$, $W(g,h)$, there are two natural ways to reduce the product of three MPOs:



(140)

By Theorem 22, there exists a complex scalar $\lambda(g,h,k) \in \mathbb{C}$ such that for any sufficiently long chain,



(141)

We show now that this scalar λ forms a three-cocycle due to associativity of the product. For the fixed reductions $V(g,h)$ and $W(g,h)$, denote the l.h.s. of Eq. (141) as $[g[hk]]$, the r.h.s. as $[[gh]k]$. Consider a product of four MPOs, $ghkl$, and the following sequence of reductions:

$$[[[gh]k]l] \to [[gh][kl]] \to [g[h[kl]]] \to [g[[hk]l]] \to [[g[hk]]l] \to [[[gh]k]l]. \tag{142}$$

In this sequence, every member can be transformed to the next by changing the reduction of three consecutive group elements. Therefore, every member is related to the previous one by a scalar. Writing out these scalars, we obtain

$$[[[gh]k]l] = \underbrace{\lambda(gh,k,l)^{-1} \cdot \lambda(g,h,kl)^{-1} \cdot \lambda(h,k,l) \cdot \lambda(g,hk,l) \cdot \lambda(g,h,k)}_{=1} \cdot [[[gh]k]l]. \tag{143}$$

As this relation is the defining relation for the three-cocycles, $\lambda : G^3 \to \mathbb{C}^*$ is a three-cocycle, where G acts trivially on $\mathbb{C}^*$.

Note that the above construction depends on the fixed reductions $V(g,h), W(g,h)$ of the product of two operators. In general, changing the reduction also changes the scalar. This change, however, is not arbitrary: we prove now that it forms a three-coboundary. Consider another reduction $\tilde{V}(g,h)$ and $\tilde{W}(g,h)$ with corresponding three-cocycle $\tilde{\lambda}$. Then, denoting the reduction with $\tilde{V}(g,h)$ and $\tilde{W}(g,h)$ by round brackets (in the sense as above), using Theorem 22,

$$(gh) = \omega(g,h)[gh] \tag{144}$$

for some $\omega(g,h) \in \mathbb{C}$. Therefore, the two scalars λ and $\tilde{\lambda}$ are related as follows:

$$((gh)k) = \omega(g,h)\omega(gh,k)[[gh]k] \tag{145}$$

$$(g(hk)) = \omega(h,k)\omega(g,hk)[g[hk]]. \tag{146}$$

Therefore, the relation between λ and $\tilde{\lambda}$ is

$$\tilde{\lambda}(g,h,k) = \frac{\omega(g,h)\omega(gh,k)}{\omega(h,k)\omega(g,hk)}\lambda(g,h,k) \tag{147}$$

This is the defining relation of three-coboundaries, thus $\lambda/\tilde{\lambda} : G^3 \to \mathbb{C}^*$ is a three-coboundary. Therefore, λ, by construction, is a three-cocycle defined up to a three-coboundary, thus, by the definition of the cohomology group, it is an element from $H^3(G,\mathbb{C}^*)$.

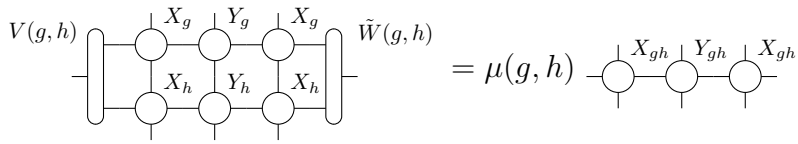
Next, consider MPO representations that are translationally invariant after blocking two tensors X and Y. The previous method assigns two possibly different labels from $H^3(G,\mathbb{C}^*)$ to the two MPO tensors XY and YX. We will show now that these two labels are in fact equal.

Proposition 23. *Let $V_n(X_gY_g)$ be a one-block projective MPO representation of G. Then $V_n(Y_gX_g)$ is also a one-block projective MPO representation of G and their third cohomology label is the same.*

Proof. As $V_n(Y_gX_g)$ is the same MPO as $V_n(X_gY_g)$, but shifted by one lattice site, it is a one-block projective MPO representation. W.l.o.g, one can suppose that both X_gY_g and Y_gX_g are injective: they contain only one block, thus they can be reduced to injective MPOs. Thus, incorporating the reductions into X_g and Y_g, we obtain two new tensors such that both X_gY_g and Y_gX_g are injective.

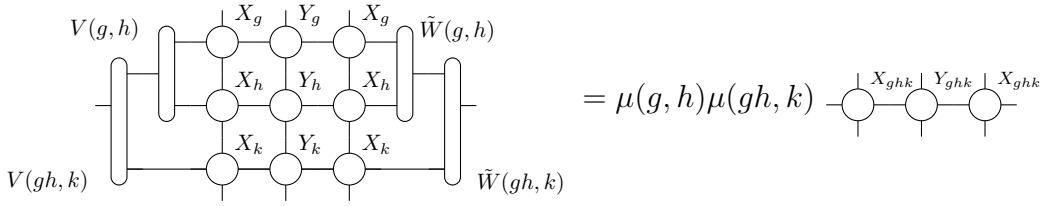
Let $V(g,h)$ and $W(g,h)$ be reductions corresponding to the product of X_gY_g and X_hY_h, while $\tilde{V}(g,h)$ and $\tilde{W}(g,h)$ be reductions for the product of Y_gX_g and X_hY_h. Then Proposition 29 in Appendix B implies that $V(g,h)$ and $\tilde{W}(g,h)$ reduces (up to a scalar) a chain of

odd number of MPO tensors:



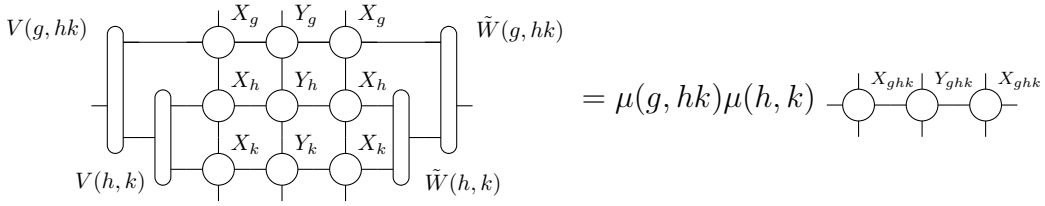
(148)

Therefore, for the product of three MPOs corresponding to g, h and k and a chain consisting of an odd number of MPO tensors,



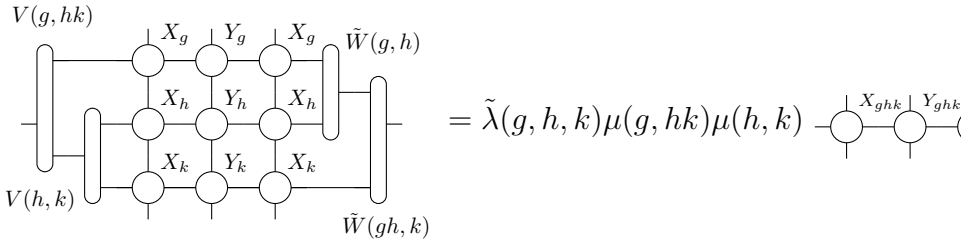
(149)

Similarly,



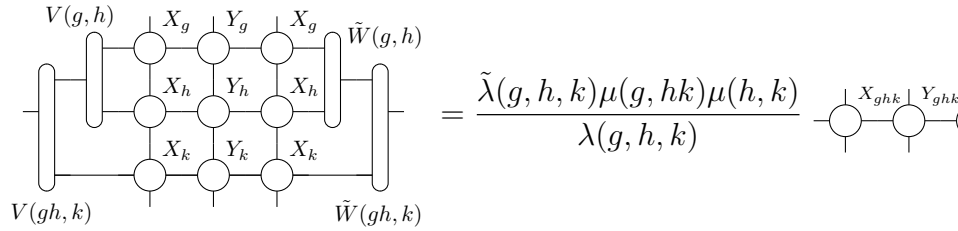
(150)

If the above chain is long enough, changing the order of the reductions $\tilde{W}$ changes the above equation only by a scalar $\tilde{\lambda}(g,h,k)$:



. (151)

Similarly, changing the order of the reductions on the left side, we get (notice that the scalar associated to changing the order of the reductions on the left side is the inverse of that on the right side, see Theorem 22)



. (152)

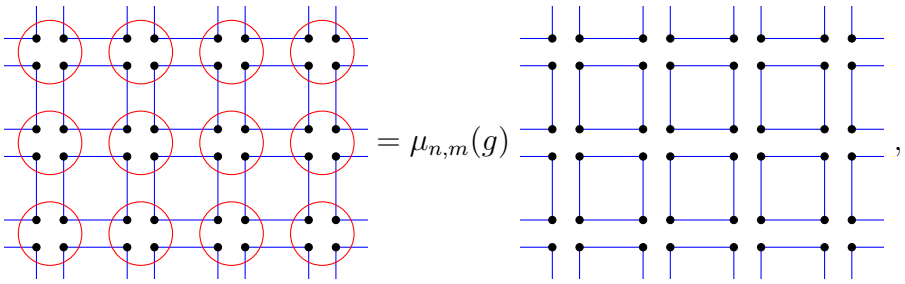
Comparing this equation with Eq. (149), we conclude that

$$\frac{\lambda(g,h,k)}{\tilde{\lambda}(g,h,k)} = \frac{\mu(g,hk)\mu(h,k)}{\mu(g,h)\mu(gh,k)} \,. \tag{153}$$

Therefore, the two scalars differ only by a three coboundary. That is, the two third cohomology labels corresponding to $X_g Y_g$ and $Y_g X_g$ coincide. □

B. Third cohomology labeling of quasi-injective PEPS

We investigate the following setup. Let G be a group, O_g a faithful (not necessarily unitary) representation of G. Let $|\phi\rangle$ be a four-partite state with full rank one-particle reduced densities. Suppose $\forall g \in G$, O_g is a symmetry of the quasi-injective PEPS defined by $|\phi\rangle$ and Id:



(154)

where the blue squares represent $|\phi\rangle$, the red operators O_g.

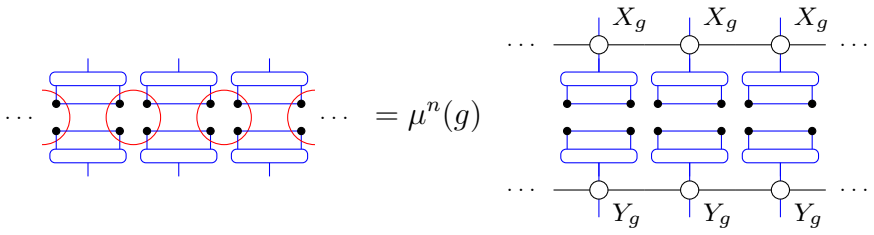
Note that this setup can readily be applied for unitary symmetries of quasi-injective PEPS: let the quasi-injective PEPS be defined by the four-partite state $|\phi\rangle$ and an invertible operator A. Let the unitary representation of the symmetry group G be U_g. Then, by inverting A in the symmetry condition, we arrive to Eq. (154) with $O_g = A^{-1}U_g A$.

Proposition 24. *If Eq.* (154) *holds for some* $n, m \geq 3$*, then it holds for all* n, m *and* $\mu_{n,m}(g) = \mu^{nm}(g)$ *for some one-dimensional representation* μ *of* G*.*

Proof. Apply Proposition 12 and notice that μ is a representation. □

We show now that the action of the symmetries show up on the boundary as a projective MPO representation of the group G.

Proposition 25. *If Eq.* (154) *holds, then for every* $g \in G$ *there are two MPO tensors* X_g *and* Y_g *such that*



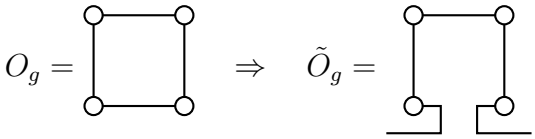
(155)

and $V_n(Y_g) = (V_n(X_g))^{-1}$ *for all* n. *Moreover,* $V_n(X_g)$ *and* $V_n(Y_g)$ *form projective representations of* G *with* $V_n(X_g)V_n(X_h) = \lambda^n(g,h)V_n(X_gX_h)$ *for a two-cocycle* λ. *In particular,* $V_n(X_g)V_n(X_h)$ *has only one block in its canonical form.*

Proof. From Theorem 13, the existence of X_g and Y_g is clear. From Corollary 14.1, it is also true that $V_n(X_g)V_n(X_h) = \lambda^n(g,h)V_n(X_gX_h)$. Due to associativity, $\lambda(g,h)\lambda(gh,k) = \lambda(g,hk)\lambda(h,k)$, and thus λ forms a two-cocycle. □

Note that if we allow for blocking, there is a length scale K for which $\lambda^{Kn}(g,h)$ becomes constant 1. On the other hand, the labeling with an element from the third cohomology group $H^3(G,\mathbb{C})$ corresponding to the $g \mapsto X_g$ one-block projective MPO representation of G is a scale-invariant labeling.

In the following, we show that the classification of the boundary MPO representation $V_n(X_g)$ also shows up in the MPO defined by O_g. To see this, we define a translationally invariant (on four sites) MPO from O_g that we call $V_n(\tilde{O}_g)$. Write O_g as an MPO in Eq. (104), and open one of the indices. We call this tensor $\tilde{O}_g$. Pictorially,

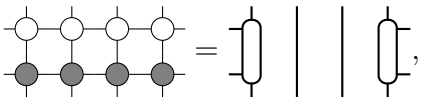


(156)

This MPO plays an important role in the third cohomology labeling of quasi-injective PEPS.

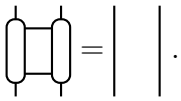
Proposition 26. *The MPOs* $V_n(\tilde{O}_g)$ *form a one-block projective MPO representation of* G. *Its third cohomology label is the same as that of* $V_n(X_g)$.

Proof. As the product of the Schmidt vectors of O_g and O_g^{-1} factorizes, the tensor $\sum_j \tilde{O}_g^{ij}\tilde{O}_{g^{-1}}^{jk}$ has the following structure:



(157)

with

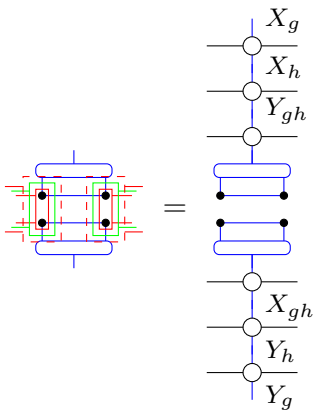


(158)

Therefore, $V_n(\tilde{O}_g)V_n(\tilde{O}_{g^{-1}}) = \mathrm{Id}$, as it is the n-fold product of this tensor.

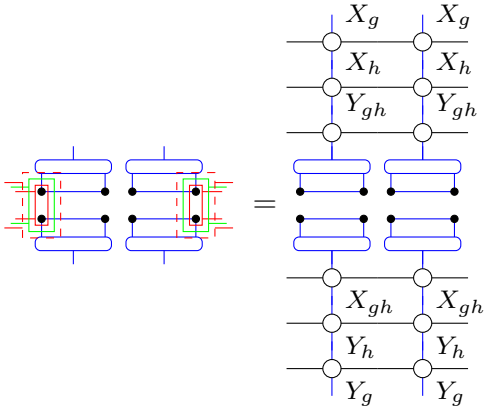
We prove now that $V_n(\tilde{O}_g)V_n(\tilde{O}_h)V_n(\tilde{O}_{(gh)^{-1}}) = \mathrm{Id}$, and thus $V_n(\tilde{O}_g)V_n(\tilde{O}_h) = V_n(\tilde{O}_{gh})$.

Consider the MPS tensor defined by the Schmidt vectors of O_g, O_h and then $O_{(gh)^{-1}}$ acting on the Schmidt vectors of $|\phi\rangle$. Then, similar to Eq. (98), this tensor can be written as



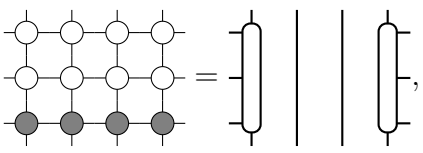
(159)

where the red solid rectangle denotes the Schmidt vectors of O_g, the green one that of O_h, and the dashed one that of $O_{(gh)^{-1}}$. Joining two such tensors, the middle operator is $O_g O_h O_{(gh)^{-1}} = \mathrm{Id}$, so



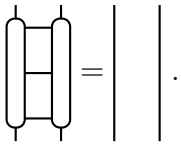
(160)

As the l.h.s. factorizes w.r.t. the vertical cut, and the r.h.s. factorizes w.r.t. the horizontal cut, and the one particle reduced densities of $|\phi\rangle$ are full rank, the product of the Schmidt vectors of O_g, O_h and $O_{(gh)^{-1}}$ also factorizes, and thus



(161)

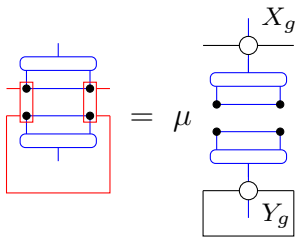
with



(162)

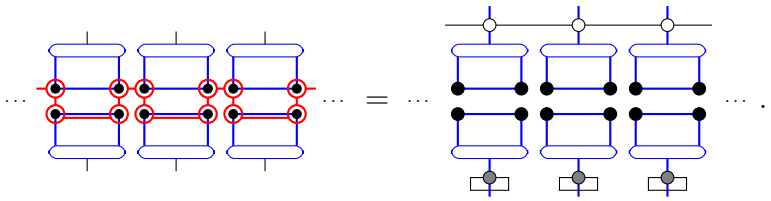
Therefore $V_n(\tilde{O}_g)V_n(\tilde{O}_h)V_n(\tilde{O}_{(gh)^{-1}}) = \mathrm{Id}$, as it is the n-fold product of this tensor. This means that $V_n(\tilde{O}_g)$ is an MPO representation.

As an MPO representation is also a one-block projective MPO representation, one can label this MPO representation with an element from the third cohomology group $H^3(G, \mathbb{C}^*)$. We now show that this label coincides with that of the projective MPO representation of G on the boundary. To see this, partially contract the MPS tensors describing the boundary of the state (defined in Eq. (95)). That is, contract only the lower indices:



(163)

Notice that the red MPO tensor acting on the l.h.s. is exactly $\tilde{O}_g$. After contracting these tensors, Eq. (163) reads



(164)

By construction, the red MPO appearing on the l.h.s. is $V_n(\tilde{O}_g)$. Therefore, if $V(g,h)$,$W(g,h)$ is a reduction from $V_n(\tilde{O}_g)V_n(\tilde{O}_h)$ to $V_n(\tilde{O}_{gh})$, then it is also a reduction from $V_n(X_g)V_n(X_h)$ to $V_n(X_{gh})$. As the third cohomology is assigned to the MPO representation with the help of these reductions, $V_n(O_g)$ is classified by the same third cohomology class as $V_n(X_g)$. □

The above proof can be repeated for the vertical boundary instead of the horizontal one. This means that the third cohomology label of the vertical boundary is the same as that of $V_n(\tilde{O}'_g)$, where $\tilde{O}'_g = D_g A_g B_g C_g$, if $O_g = A_g B_g C_g D_g$. Proposition 23 implies that the third cohomology labeling of $V_n(\tilde{O}'_g)$ and $V_n(\tilde{O}_g)$ coincide, therefore the third cohomology labeling of the horizontal and vertical boundary coincide.

VIII. CONCLUSION

In this work we introduced a new class of PEPS, quasi-injective PEPS. We showed that quasi-injective PEPS are a generalization of injective PEPS and that some important examples that are not known to have an injective PEPS description naturally admit a quasi-injective PEPS description. We showed that they are unique ground state of their parent Hamiltonian. We also derived a canonical form, i.e., a way to decide locally if two quasi-injective PEPS are equal. One of the necessary conditions is that the boundaries of the two states are related by an invertible MPO. Using this result, the third cohomology labeling of SPT phases extends naturally to quasi-injective PEPS, suggesting that these states are appropriate to capture the relevant physics of SPT phases. Using the canonical form, we have found that the third cohomology label of the SPT phase is not only encoded on the edge of the model, but also directly in the symmetry operators.

IX. ACKNOWLEDGEMENTS

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Appendix A: Examples for canonical form

In the injective PEPS case, if two tensors generate the same state, then they are related by a product gauge transformation. In the case of quasi-injective PEPS, this is no longer true as the following example shows.

Let A be the following MPS tensor:

$$A^0 = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \tag{A1}$$

$$A^1 = \begin{pmatrix} 24 & -10 \\ 17 & -3 \end{pmatrix}. \tag{A2}$$

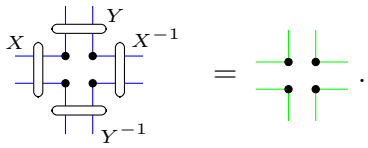
This tensor was constructed in such a way that it is Z symmetric for size 4, but not for longer chains: for the tensor B with $B^0 = A^0$ and $B^1 = -A^1$, $V_4(B) = V_4(A)$, but $V_5(A) \neq V_5(B)$.

The tensors A and B are also normal, after blocking two tensors they become injective. Proposition 7 also implies that A and B are not related by a gauge transform. There is also no gauge relating the tensors after blocking four of them: $\nexists X:\ XBBBBX^{-1} = AAAA$.

Consider two quasi-injective PEPS. Let Ψ_A be defined by $\phi_A = V_4(A)$ and Id, Ψ_B by $\phi_B = V_4(B)$ and Id. By construction, $\Psi_A = \Psi_B$. We will show, however, that the PEPS tensors defined by grouping four MPS tensors:

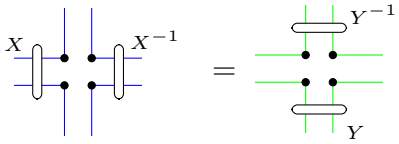
(A3)

are not related by a gauge, where the blue tensors are A and the green ones are B. We prove that by contradiction. Suppose there are such gauges, X and Y:



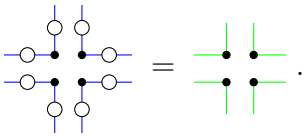
(A4)

Inverting Y and Y^{-1}, we get that



(A5)

Notice that the l.h.s. is product w.r.t. the vertical cut, whereas the r.h.s. is product w.r.t. the horizontal cut. As A and B become injective after blocking two tensors, both X and Y have to be product operators, and thus



(A6)

But this would mean that after blocking four tensors, $BBBB = XAAAAX^{-1}$ for some gauge X. As this is a contradiction, the two given PEPS tensors generating the same quasi-injective PEPS are not related by a gauge.

Appendix B: MPS reductions

In this Section, we present the proofs of the theorems about reductions of MPS used in Section VII.

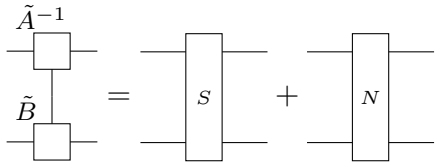
Proposition 20. *Let A be a normal MPS tensor, B an MPS tensor such that for some $\lambda \in \mathbb{C}$*

$$V_n(B) = \lambda^n V_n(A) \quad \forall n \in \mathbb{N}. \tag{135}$$

Then there exist matrices V, W such that $VW = \mathrm{Id}$ and $\forall n \in \mathbb{N}$ and $(i_1, i_2 \dots i_n) \in \{1, 2, \dots d\}^n$,

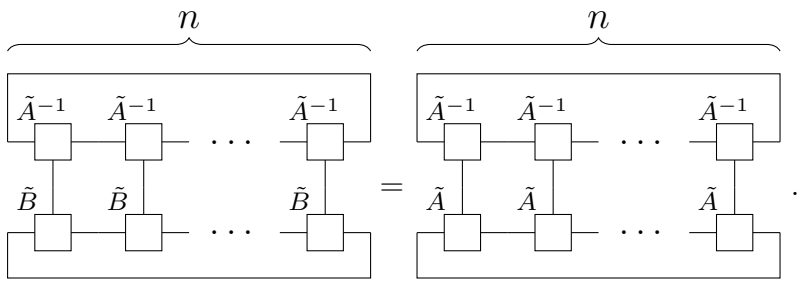
$$V B^{i_1} \dots B^{i_n} W = A^{i_1} \dots A^{i_n} \tag{136}$$

Proof. Suppose the injectivity length (see Proposition 5) of A is L. Let $\tilde{A}$ and $\tilde{B}$ denote the tensors obtained from A and B by blocking them L times, respectively. Then $\tilde{A}$ has a left inverse, $\tilde{A}^{-1}$. Take the Jordan decomposition of the following matrix:



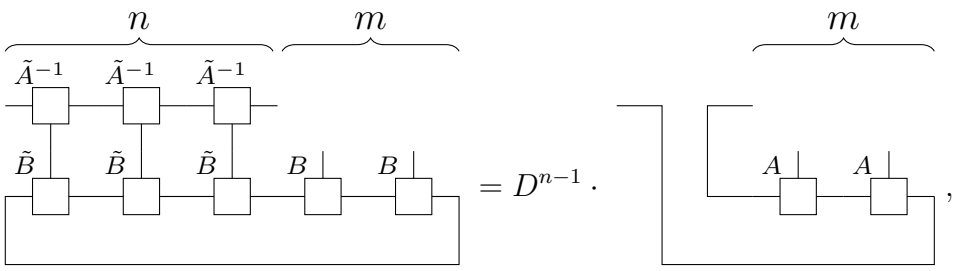
(B1)

where S is semi-simple (diagonalizable), N is nilpotent (upper triangular in the basis in which S is diagonal) and $[S, N] = 0$. B and A generate the same state, thus



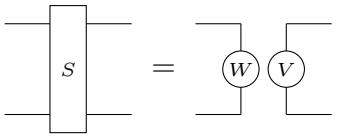
(B2)

The r.h.s is D^n, where D is the bond dimension of A, as it is n times the trace of Id. Using the Jordan decomposition Eq. (B1), the l.h.s. is $\mathrm{Tr}(S + N)^n = \mathrm{Tr}\, S^n$. Therefore $\mathrm{Tr}\, S^n = D^n$, thus Proposition 10 implies that the rank of S is 1. $[S, N] = 0$ therefore implies that $SN = NS = 0$. Thus, $(S + N)^n = S^n + N^n = S^n$ if n is larger than the nilpotency rank of N. Then, as A and B generate the same state, for all n and m,



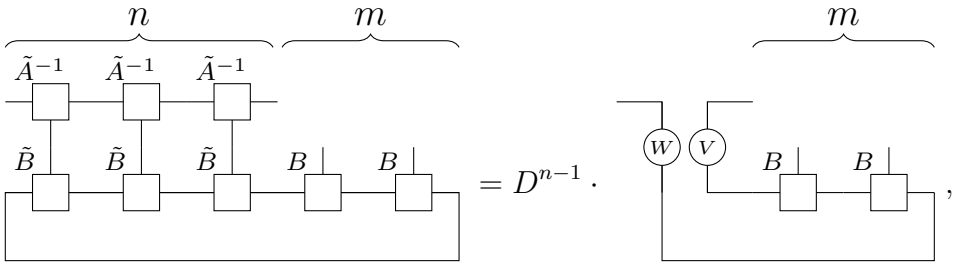
(B3)

where we have used $n-1$ times that $\operatorname{Tr}\mathrm{Id} = D$. As S is rank one, there are matrices V and W such that S can be written as



(B4)

Therefore, as $N^n = 0$, the l.h.s. can be rewritten as



(B5)

Therefore, comparing this with the r.h.s. of Eq. (B3), for all m,

$$VB^{i_1}\dots B^{i_m}W = A^{i_1}\dots A^{i_m}. \tag{B6}$$

For $m = 0$, $VW = \mathrm{Id}$. □

Proposition 21. *Let V, W be a reduction from B to A. Let $N^i = B^i - WA^iV$. Then the algebra generated by N^i is nilpotent.*

Before proceeding to the proof, we need the following simple statement:

Lemma 27. *Let V, W be a reduction from B to an injectie MPS tensor A, $N^i = B^i - WA^iV$. Then for any $m > 0$,*

$$VN^{i_1}N^{i_2}\dots N^{i_m}W = 0. \tag{B7}$$

Proof. We prove this by induction on m. For $m = 1$,

$$VN^iW = VB^iW - VWA^iVW = A^i - A^i = 0. \tag{B8}$$

Suppose the statement is true for all $n < m$. Then, writing $N^{i_1} = B^{i_1} - WA^{i_1}V$ and using the induction hypothesis,

$$VN^{i_1}N^{i_2}\dots N^{i_m}W = VB^{i_1}N^{i_2}\dots N^{i_m}W \tag{B9}$$

Similarly, $N^{i_2}, \dots, N^{i_{m-1}}$ can be changed to $B^{i_2}, \dots, B^{i_{m-1}}$:

$$VN^{i_1}N^{i_2}\dots N^{i_m}W = VB^{i_1}\dots B^{i_{m-1}}N^{i_m}W. \tag{B10}$$

Writing now $N^{i_m} = B^{i_m} - WA^{i_m}V$, we arrive to

$$VN^{i_1}\dots N^{i_m}W = VB^{i_1}\dots B^{i_m}W - VB^{i_1}\dots B^{i_{m-1}}WA^{i_m}VW = 0. \tag{B11}$$

□

Proof of Proposition 21. B and A generate the same state:

$$\mathrm{Tr}\left\{B^{i_1}B^{i_2}\dots B^{i_n}\right\} = \mathrm{Tr}\left\{A^{i_1}A^{i_2}\dots A^{i_n}\right\}. \tag{B12}$$

Write $B^i = WA^iV + N^i$ and expand the product on the l.h.s. As V and W form a reduction, $VN^{i_1}\dots N^{i_m}W = 0$ for any $m > 0$ and all $i_1, \dots i_m$ by Lemma 27, and thus all terms cancel except the products of A and the products of N. Therefore

$$\mathrm{Tr}\left\{N^{i_1}N^{i_2}\dots N^{i_n}\right\} = 0. \tag{B13}$$

This means that $\mathrm{Tr}\{Z\} = 0$ for every element Z in the algebra generated by N^i. Thus, in particular, for every $n > 0$, $\mathrm{Tr}\{Z^n\} = 0$. Therefore the algebra generated by N^i is a nil algebra, and thus nilpotent[49]. That is,

$$N^{i_1}N^{i_2}\dots N^{i_n} = 0 \tag{B14}$$

for large enough n. □

Theorem 22. *Let V, W and $\tilde{V}, \tilde{W}$ be two reductions from B to a normal tensor A. Let the nilpotency length of both reductions be at most N_0. Then $\exists\lambda \in \mathbb{C}$ such that for any $n > 2N_0$,*

$$VB^{i_1}B^{i_2}\dots B^{i_n} = \lambda\tilde{V}B^{i_1}B^{i_2}\dots B^{i_n} \tag{138}$$

$$B^{i_1}B^{i_2}\dots B^{i_n}W = \lambda^{-1}B^{i_1}B^{i_2}\dots B^{i_n}\tilde{W}. \tag{139}$$

Before proceeding to the proof, we need the following calculation that we use repeatedly:

Lemma 28. *Let V, W be a reduction from B to a normal tensor A, $N^i = B^i - WA^iV$. Let N_0 be the nilpotency length of the reduction. Then the following equations hold:*

$$B^{i_1}B^{i_2}\dots B^{i_n} = \sum_{0\le k\le l\le n} N^{i_1}\dots N^{i_k}WA^{i_{k+1}}\dots A^{i_l}VN^{i_{l+1}}\dots N^{i_n} \tag{B15}$$

$$VB^{i_1}B^{i_2}\dots B^{i_n} = \sum_{\max(0,n-N_0)\le l\le n} A^{i_1}\dots A^{i_l}VN^{i_{l+1}}\dots N^{i_n} \tag{B16}$$

$$B^{i_1}B^{i_2}\dots B^{i_n}W = \sum_{0\le k\le \min(N_0,n)} N^{i_1}\dots N^{i_k}WA^{i_{k+1}}\dots A^{i_n}. \tag{B17}$$

Proof. Write $B^{i_j} = WA^{i_j}V + N^{i_j}$ for all j in $B^{i_1} \dots B^{i_n}$ and expand the expression. Using Lemma 27 and the definition of the nilpotency length (Definition 8), we arrive at the desired equations. □

Proof of Theorem 22. Let L be the injectivity length of A and let $m = 2N_0 + L$. Consider

$$C^{i_1 \dots i_m} = VB^{i_1}B^{i_2} \dots B^{i_m}\tilde{W}. \tag{B18}$$

Using Lemma 28 with $B^i = WA^iV + N^i$, we have

$$C^{i_1 \dots i_m} = \sum_{k=N_0+L}^{m} A^{i_1} \dots A^{i_k} V N^{i_{k+1}} \dots N^{i_m} \tilde{W}, \tag{B19}$$

as $m - N_0 = N_0 + L$. Similarly, using Lemma 28 with $B^i = \tilde{W}A^i\tilde{V} + \tilde{N}^i$, we get

$$C^{i_1 \dots i_m} = \sum_{k=0}^{N_0} V\tilde{N}^{i_1} \dots \tilde{N}^{i_k} \tilde{W} A^{i_{k+1}} \dots A^{i_m}. \tag{B20}$$

Note that the MPS tensor at position $k = N_0 + 1$ to $N_0 + L$ is A^{i_k} in both expressions. By assumption, that block is injective. Applying its inverse and comparing the two expressions, we conclude that

$$\sum_{k=0}^{N_0} V\tilde{N}^{i_1} \dots \tilde{N}^{i_k} \tilde{W} A^{i_{k+1}} \dots A^{i_{N_0}} = \lambda A^{i_1} \dots A^{i_{N_0}} \tag{B21}$$

$$\sum_{k=0}^{N_0} A^{i_1} \dots A^{i_k} V N^{i_{k+1}} \dots N^{i_{N_0}} \tilde{W} = \lambda^{-1} A^{i_1} \dots A^{i_{N_0}} \tag{B22}$$

for some $\lambda \in \mathbb{C}$. But then, using Lemma 28 for $VB^{i_1}B^{i_2} \dots B^{i_n}$ with $B^i = \tilde{W}A^i\tilde{V} + \tilde{N}^i$, we get

$$VB^{i_1}B^{i_2} \dots B^{i_n} = \sum_{k=0}^{N_0} \sum_{l=n-N_0}^{n} V\tilde{N}^{i_1} \dots \tilde{N}^{i_k} \tilde{W} A^{i_{k+1}} \dots A^{i_l} \tilde{V} N^{i_{l+1}} \dots N^{i_n}. \tag{B23}$$

If $n \geq 2N_0$, then $l \geq N_0$. Therefore the left part of the r.h.s. can be replaced using Eq. (B21):

$$VB^{i_1}B^{i_2} \dots B^{i_n} = \lambda \sum_{l=n-N_0}^{n} A^{i_1} \dots A^{i_l} \tilde{V} N^{i_{l+1}} \dots N^{i_n} = \lambda \tilde{V} B^{i_1} B^{i_2} \dots B^{i_n}, \tag{B24}$$

where the last equation holds by using Lemma 28 for $\tilde{V}B^{i_1}B^{i_2} \dots B^{i_n}$ with $B^i = \tilde{W}A^i\tilde{V} + \tilde{N}^i$. Equation (139) can be proven similarly using Eq. (B22). □

We now consider MPSs that are translationally invariant after blocking two sites.

Proposition 29. *Let $A \in \mathbb{C}^{D_1} \otimes \mathbb{C}^{D_2} \otimes \mathbb{C}^{d_1}$ and $B \in \mathbb{C}^{D_2} \otimes \mathbb{C}^{D_1} \otimes \mathbb{C}^{d_2}$ be two tensors such that both AB and BA are normal MPS tensors. Let $C \in \mathbb{C}^{\tilde{D}_1} \otimes \mathbb{C}^{\tilde{D}_2} \otimes \mathbb{C}^{d_1}$ and $D \in \mathbb{C}^{\tilde{D}_2} \otimes \mathbb{C}^{\tilde{D}_1} \otimes \mathbb{C}^{d_1}$ be two tensors such that $V_n(CD) = V_n(AB)$. Then $V_n(BA) = V_n(DC)$ and if V, W are reductions of CD to AB and $\tilde{V}, \tilde{W}$ are reductions of DC to BA, then for a sufficiently long chain,*

$$AB \dots BA = \lambda VCD \dots DC\tilde{W} \tag{B25}$$

$$BA \dots AB = \mu \tilde{V} DC \dots CDW \tag{B26}$$

Proof. First, notice that $V_n(BA) = V_n(DC)$, as $V_n(BA)$ is $V_n(AB)$ shifted by half a lattice constant, while $V_n(DC)$ is $V_n(CD)$ shifted by half a lattice constant.

Next, using Lemma 28 with $CD = WABV + N_1 N_2$, we have

$$V \underbrace{CD \dots D}_{2k} C\tilde{W} = \sum_{i=0}^{M} \underbrace{AB \dots B}_{2k-2i} V \underbrace{N_1 N_2 \dots N_1 N_2}_{2i} C\tilde{W}, \tag{B27}$$

where M is the injectivity length of the reduction V, W. Similarly, using Lemma 28 with $DC = \tilde{W}BA\tilde{V} + \tilde{N}_1 \tilde{N}_2$, we have

$$VC \underbrace{D \dots DC}_{2k} \tilde{W} = \sum_{i=0}^{\tilde{M}} VC \underbrace{\tilde{N}_1 \tilde{N}_2 \dots \tilde{N}_1 \tilde{N}_2}_{2i} \tilde{W} \underbrace{BA \dots BA}_{2k-2i}, \tag{B28}$$

Where $\tilde{M}$ is the injectivity length of $\tilde{V}, \tilde{W}$. Therefore, if $2k > 2M + 2\tilde{M} + 2L$, where L is the injectivity length of AB, then

$$V \underbrace{CD \dots C}_{2k+1} \tilde{W} = \underbrace{AB \dots A}_{2N+1} \underbrace{B \dots A}_{2k-1-2N} \underbrace{\square}_{2N+1} = \underbrace{\square}_{2N+1} \underbrace{B \dots A}_{2k-1-2N} \underbrace{B \dots A}_{2N+1} \tag{B29}$$

As the middle part is injective, the last equation can hold only if $AB \dots BA = \lambda VCD \dots DC\tilde{W}$. The other equation can be proven similarly. □

Appendix C: The qubit case

In this section, we characterize how two quasi-injective PEPS defined by $(|\phi_A\rangle, O)$ and $(|\phi_B\rangle, \mathrm{Id})$ with $|\phi_A\rangle, |\phi_B\rangle \in (\mathbb{C}^2)^{\otimes 4}$ can generate the same state. We restrict ourselves to the case where $|\phi_A\rangle$ and $|\phi_B\rangle$ do not factorize in either direction. Using Corollary 18.1, $|\phi_A\rangle$ and $|\phi_B\rangle$ are SLOCC equivalent, and thus we can suppose $|\phi_A\rangle = |\phi_B\rangle$ (by changing O).

Notice that the state $|\xi\rangle$ appearing in the proof of Theorem 18 (see Eq. (125)) is also SLOCC equivalent with ϕ_A. We can thus suppose that $|\phi_A\rangle = |\phi_B\rangle = |\xi\rangle$. Therefore, given $|\phi_A\rangle$, we only need to characterize all pairs of two-body invertible operators such that Eq. (125) holds.

Let us fix $|\phi_A\rangle = |\phi_B\rangle = |\xi\rangle$. We start the investigation with a state such that in the horizontal cut it has Schmidt rank two. As the span of the Schmidt vectors contains a product state and we are only interested in $|\phi_A\rangle$ up to SLOCC equivalence, w.l.o.g. we can suppose that a basis of its reduced density on the upper two particles is

$$|\Psi_1\rangle = |00\rangle \tag{C1}$$

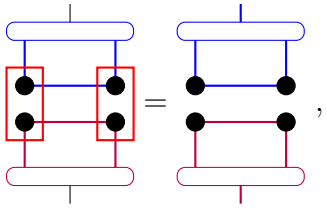
$$|\Psi_2\rangle = a|01\rangle + b|10\rangle + c|11\rangle, \tag{C2}$$

whereas a basis of its reduced density on the lower two particles is

$$|\Phi_1\rangle = |00\rangle \tag{C3}$$

$$|\Phi_2\rangle = A|01\rangle + B|10\rangle + C|11\rangle\ . \tag{C4}$$

In this setting, we are looking for invertible two body operators O_1 and O_2 such that



(C5)

where the left red rectangle represents O_1, the right one O_2, while the blue Schmidt vectors are $\Psi_{1/2}$, the purple ones are $\Phi_{1/2}$. This gives four times sixteen equations on the matrix elements of O_1 and O_2. Checking these equations can be done in any CAS. The following cases can be distinguished.

- $C \neq 0$, $c \neq 0$. In this case, the operators are (α, β, γ are free parameters):

$$\begin{aligned} O_1 =& |00\rangle\langle 00| + \alpha|01\rangle\langle 01| + \frac{b}{c}(\alpha-1)|00\rangle\langle 01| + \beta|10\rangle\langle 10| + \frac{B}{C}(\beta-1)|00\rangle\langle 10| + \\ & \gamma|11\rangle\langle 11| + \frac{b}{c}(\gamma-\beta)|10\rangle\langle 11| + \frac{B}{C}(\gamma-\alpha)|01\rangle\langle 11| + \frac{Bb}{Cc}(1+\gamma-\alpha-\beta)|00\rangle\langle 11| \end{aligned} \tag{C6}$$

$$\begin{aligned} O_2 =& |00\rangle\langle 00| + \frac{1}{\alpha}|01\rangle\langle 01| + \frac{a}{c}(\frac{1}{\alpha}-1)|00\rangle\langle 01| + \frac{1}{\beta}|10\rangle\langle 10| + \frac{A}{C}(\frac{1}{\beta}-1)|00\rangle\langle 10| + \\ & \frac{1}{\gamma}|11\rangle\langle 11| + \frac{a}{c}(\frac{1}{\gamma}-\frac{1}{\beta})|10\rangle\langle 11| + \frac{A}{C}(\frac{1}{\gamma}-\frac{1}{\alpha})|01\rangle\langle 11| + \frac{aA}{Cc}(1+\frac{1}{\gamma}-\frac{1}{\alpha}-\frac{1}{\beta})|00\rangle\langle 11| \end{aligned} \tag{C7}$$

- $C \neq 0$, $c = 0$. In this case $b \neq 0$, otherwise the one particle reduced densities of the state is not full rank. The operators are (α, β, γ are free parameters):

$$\begin{aligned} O_1 =& |00\rangle\langle 00| + |01\rangle\langle 01| + \alpha|00\rangle\langle 01| + \beta|10\rangle\langle 10| + \frac{B}{C}(\beta-1)|00\rangle\langle 10| + \\ & \beta|11\rangle\langle 11| + \gamma|10\rangle\langle 11| + \frac{B(\beta-1)}{C}|01\rangle\langle 11| + \frac{B\gamma - B\alpha}{C}|00\rangle\langle 11| \end{aligned} \tag{C8}$$

$$\begin{aligned} O_2 =& |00\rangle\langle 00| + |01\rangle\langle 01| - \frac{a}{b}\alpha|00\rangle\langle 01| + \frac{1}{\beta}|10\rangle\langle 10| + \frac{A}{C}(\frac{1}{\beta}-1)|00\rangle\langle 10| + \\ & \frac{1}{\beta}|11\rangle\langle 11| - \frac{a\gamma}{b\beta^2}|10\rangle\langle 11| + (-\frac{A}{C} + \frac{A}{C\beta})|01\rangle\langle 11| + \frac{Aa\gamma - Aa\gamma/\beta^2}{Cb}|00\rangle\langle 11| \end{aligned} \tag{C9}$$

- $c = 0$, $C = 0$. In this case $B \neq 0, b \neq 0$, otherwise the one particle reduced densities of the state is not full rank. The operators are (α, β, γ are free parameters):

$$\begin{aligned} O_1 =& |00\rangle\langle 00| + |01\rangle\langle 01| + \alpha|00\rangle\langle 01| + |10\rangle\langle 10| + \beta|00\rangle\langle 10| + \\ & |11\rangle\langle 11| + \alpha|10\rangle\langle 11| + \beta|01\rangle\langle 11| + \gamma|00\rangle\langle 11| \end{aligned} \tag{C10}$$

$$\begin{aligned} O_2 =& |00\rangle\langle 00| + |01\rangle\langle 01| - \frac{a}{b}\alpha|00\rangle\langle 01| + |10\rangle\langle 10| - \frac{B}{A}\beta|00\rangle\langle 10| + \\ & |11\rangle\langle 11| - \frac{a}{b}\alpha|10\rangle\langle 11| - \frac{A}{B}\beta|01\rangle\langle 11| + \frac{2Aa\alpha\beta - Aa\gamma}{Bb}|00\rangle\langle 11| \end{aligned} \tag{C11}$$

Using this result, we have checked that if the state has Schmidt rank at least 3, then O_1 and O_2 can only be product operators.

To find therefore all possible operators O such that the quasi-injective PEPS defined by $(|\phi_A\rangle, O)$ and by $(|\phi_B\rangle, \mathrm{Id})$ are the same (supposing they have Schmidt rank at least two along both vertical and horizontal cut), one has to do the following steps:

1. Transform $|\phi_A\rangle$ with an invertible product operator O_1 to have $|00\rangle$ in the span of its Schmidt vectors in both the upper and lower two particles

2. If the Schmidt rank of $|\phi_A\rangle$ is two along the horizontal cut, then take the two-body operators given above, $O_2 \otimes O_3$. Otherwise take $O_2 = O_3 = \mathrm{Id}$.

3. Repeat the previous two steps for the vertical cut, giving an invertible product operator O_4 and two-body invertible operators $O_5 \otimes O_6$.

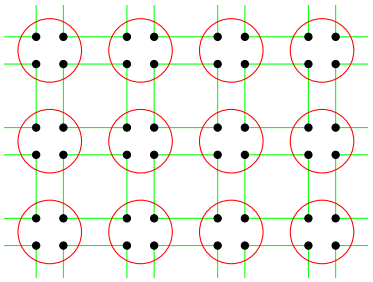
4. Find all invertible product transformation O_7 such that $|\phi_B\rangle = O_7|\phi_A\rangle$.

Then all possible operators O are given by $\tilde{O}_1(O_2 \otimes O_3)\tilde{O}_1^{-1}\tilde{O}_4(O_5 \otimes O_6)\tilde{O}_4^{-1}\tilde{O}_7$, where $\tilde{O}_i = SO_iS$, and S is the swap operator defined before Theorem 17.

Appendix D: G-injective tensors

In this section, we try to generalize quasi-injective PEPS in a way that it also includes G-injective PEPS. We try the obvious generalization: if the quasi-injective PEPS $(|\phi\rangle, \mathrm{Id})$ has symmetries O_g for $g \in G$ for some group G, then $|\phi\rangle$ and $\sum_g O_g$ defines a non-quasi-injective PEPS that could be a candidate to include G-injective PEPS. We present here, however, an example for such a state, that behaves very different from G-injective PEPS.

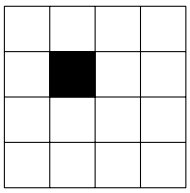
Consider the following state:

$|\Psi\rangle =$  , (D1)

where the green rectangle is a four-partite GHZ state, and the red circle is $O = \mathrm{Id} + Z^{\otimes 4}$.

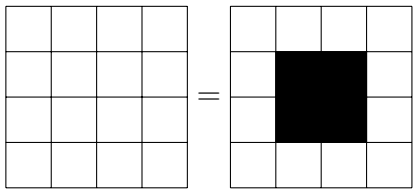
We will show that on an $n \times n$ torus, there are at least 2^n linearly independent states that are locally indistinguishable from this state. This means that given any local (frustration free) parent Hamiltonian, its ground space is at least 2^n-fold degenerate.

To see this, consider states on the torus that are constructed similar to $|\Psi\rangle$, except that some of the four-partite GHZ states $|\phi^+\rangle = 1/\sqrt{2}(|0000\rangle + |1111\rangle)$ are changed to $|\phi^-\rangle = 1/\sqrt{2}(|0000\rangle - |1111\rangle)$. Such a state will be depicted schematically as a rectangular grid, with squares colored black at all occurrence of $|\phi^-\rangle$. For example, the figure below depicts such a state with one occurrence of $|\phi^-\rangle$:

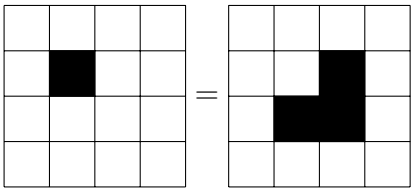
 . (D2)

We will see that these states are all locally indistinguishable from $|\Psi\rangle$ and that they span an at least $\exp\{n/2\}$-dimensional space. First notice that $|\phi^-\rangle = Z|\phi^+\rangle$, where Z acts on one of the four particles (any one of them). Due to the special form of O, however, if in a

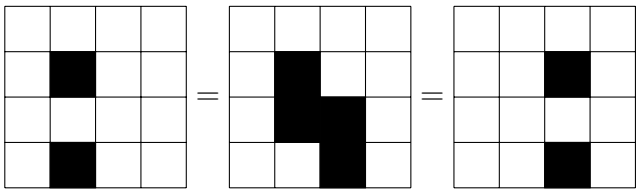
2×2 block all $|\phi^+\rangle$ are changed to $|\phi^-\rangle$, it doesn't change the state:

$|\Psi\rangle =$  . (D3)

In fact, inverting the color of all rectangles in any 2×2 rectangle doesn't change the state. For example,

 . (D4)

A consequence of this is that a pair of black rectangles in the same column (row) can "travel" horizontally (vertically) no matter how far they are separated. As an illustration, let us show how to move two black rectangles in the same column separated by one to the neighboring column:

 . (D5)

This means that these states are indistinguishable from $|\Psi\rangle$ on any finite (system size independent) region. Inverting the color of all rectangles in any 2×2 rectangle in fact defines an equivalence relation on the colorings of the grid: two colorings are equivalent if and only if they can be transformed to each other by repeatedly inverting the color of all rectangles in 2×2 regions. Equivalent colorings correspond to the same state, whereas inequivalent colorings to perpendicular ones: such states all have the form $(1 + Z^{\otimes 4})^{\otimes n} |\phi^\pm\rangle^{\otimes n}$. Expanding this expression, we get a sum of tensor products of $|\phi^+\rangle$ and $|\phi^-\rangle$. Starting from two equivalent colorings, the sum contains the same terms reordered. Starting from inequivalent colorings, all terms differ from each other and thus the states are perpendicular as $\langle \phi^+ | \phi^- \rangle = 0$. To see that there are at least 2^n equivalence classes, notice that the parity of black rectangles in each column is an invariant. (And for each parity assignment there is a coloring with that parities.)

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3.4 Classification of MPS with a local (gauge) symmetry

In this Section we include the following paper:

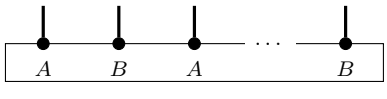
- Ilya Kull, Andras Molnar, Erez Zohar, and J. Ignacio Cirac. "Classification of Matrix Product States with a Local (Gauge) Symmetry". In: *Annals of Physics, Volume 386, November 2017, Pages 199-241* 386 (Aug. 1, 2017), pp. 199–241. arXiv: 1708.00362v2

Gauge theories provide us with the language of modern particle physics. Three out of the four fundamental interactions (electromagnetic, weak and strong, all included in the standard model of particle physics) are described by gauge theories. Moreover, they also emerge as effective low-energy descriptions in condensed matter systems. Given a field with global symmetries, the gauge principle consists of introducing extra degrees of freedom (the gauge field) such that the global symmetry becomes local. These gauge fields are then used to describe the gauge bosons (such as the photon). While weakly coupled gauge theories, such as the Abelian theory of quantum electrodynamics, are well understood by perturbative tools, non-Abelian theories pose some difficulties yet to be solved due to their low-energy non-perturbative behavior. One way around is the use of Monte Carlo methods on a discretized space-time (or in the Hamiltonian formulation, space). While these methods are very successful, they fail to describe large fermionic densities or real time evolution. Due to these difficulties Tensor Network methods to describe these lattice versions of the gauge theories are gaining popularity.

Apart from numerical simulations based on MPS and PEPS, these TN representations are useful for theoretical investigations of lattice gauge theories. This approach focuses on the states rather then the Hamiltonians: gauge invariance is required on the state level, and the corresponding parent Hamiltonian will also automatically have that symmetry. Several formulations have been proposed to describe gauge invariant TNS, all starting from a symmetric tensor describing the matter field and later on introducing an other tensor describing the gauge field such that the combined network is gauge invariant. In our investigation we try to understand what are the minimal requirements for an MPS to describe a LGT: we characterize how it can possess local (gauge) symmetries.

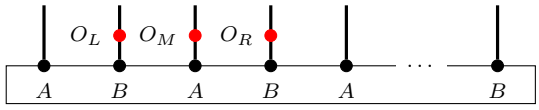
In the most general case, we consider an MPS where the odd sites (the A tensors) correspond to the matter field while the even sites (the B tensors) to the gauge field:

$$|\Psi\rangle = \quad . \tag{3.5}$$



Apart from this kind of states, we also consider MPS representing pure gauge filed and MPS representing pure matter field. We consider local symmetry operations of the form

$$O|\Psi\rangle = \quad . \tag{3.6}$$



In this paper we investigate what are the properties of the A and B tensors representing the matter and gauge fields such that the state is symmetric under these local operations: $|\Psi\rangle = O|\Psi\rangle$. We consider both finite and compact symmetry groups. We find examples where the gauge symmetry does not originate from a global symmetry of the matter field which are not included in the conventional, gauge principle setting.

The main technical challenge of this project was that the MPS description of $O|\Psi\rangle$ is non-translationally invariant. As the fundamental theorem is usually stated for translationally invariant states, one has to understand how it generalizes to this setup. This need for generalization provides a natural connection to the next Section, where we consider non-TI TNS with arbitrary lattice geometry.

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Classification of matrix product states with a local (gauge) symmetry

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HIGHLIGHTS

- Structure of tensors generating states (MPS) with local symmetry is determined.
- Three types of states analyzed: matter, pure gauge field and their combined state.
- Structure of gauge field Hilbert space derived from local symmetry assumption.
- New gauge invariant states described, not the result of gauging a global symmetry.

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ABSTRACT

Matrix Product States (MPS) are a particular type of one dimensional tensor network states, that have been applied to the study of numerous quantum many body problems. One of their key features is the possibility to describe and encode symmetries on the level of a single building block (tensor), and hence they provide a natural playground for the study of symmetric systems. In particular, recent works have proposed to use MPS (and higher dimensional tensor networks) for the study of systems with local symmetry that appear in the context of gauge theories. In this work we classify MPS which exhibit local invariance under arbitrary gauge groups. We study the respective tensors and their structure, revealing known constructions that follow known gauging procedures, as well as different, other types of possible gauge invariant states.

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1. Introduction

Gauge theories play a paramount role in modern physics. Through the gauge principle, the theories describing the fundamental interactions in the standard model of particle physics are obtained by lifting the global symmetries of the interaction-free matter theories to be local symmetries, minimally coupled [1] to a gauge field. Moreover, they also emerge as effective low-energy descriptions in several condensed matter scenarios [2]. Historically, the gauging procedure was first conceived as a transformation of a Lagrangian or Hamiltonian describing a physical system; however, it can be performed on the level of quantum states as well, irrespective of dynamics associated to a specific theory.

In spite of their central role in the standard model, non-Abelian gauge theories still involve puzzles to be solved. Their complete understanding still poses a significant challenge due to non-perturbative phenomena (e.g. low energy QCD). Among the various approaches proposed to tackle the strongly coupled regime, a particularly general and successful one is lattice gauge theory [3]. Monte Carlo sampling of Wilson's Euclidean lattice version of gauge theories has so far been the most successful method of numerical simulation, nevertheless, it suffers from its own drawbacks. The sign problem [4] prevents application to systems with large fermionic densities, and the use of Euclidean time does not allow to study real time evolution and non-equilibrium phenomena in general scenarios. In order to describe real-time evolution of such theories, one is forced to abandon the Monte Carlo approach, and search for other methods. In this context, the Hamiltonian formulation of Kogut and Susskind [5] has been receiving renewed interest, with two recent approaches coming from the quantum information and quantum optics community: quantum simulation, using optical, atomic or solid-state systems [6,7], and tensor network states.

The representation of quantum many-body states as tensor networks is connected to White's density-matrix renormalization group [8], and in the case of one dimensional spin lattices is known as matrix product states (MPS) [9]. Among many useful properties of tensor networks, one which makes them well suited to the description of states with symmetries, is the ability to encode the symmetry on the level of a single tensor (or a few) describing the state. In the case of global symmetries, both for MPS and for certain classes of PEPS in 2D (Projected Entangled Pair States — the generalization of MPS to higher dimensional lattices), the relation between the symmetry of the state and the properties of the tensor is well understood [10]. Tensor networks studies of lattice gauge theories have so far included numerical works (e.g., mass spectra, thermal states, real time dynamics and string breaking, phase diagrams etc. for the Schwinger model and others) [11–30], furthermore, several theoretical formulations of classes of gauge invariant tensor network states have been proposed [31–35]. In all of the latter the construction method follows the ones common to conventional gauge theory formulations: symmetric tensors are used to describe the matter degree of freedom, and later on a gauge field degree of freedom is added, or, alternatively - a pure gauge field theory is considered. While the usefulness of tensor networks in lattice gauge theories has certainly been demonstrated by the above mentioned works, so far there were few attempts (e.g. [13]) to generally classify tensor network states with local symmetry.

In this paper, starting from the assumption of a local symmetry, we find necessary and sufficient conditions to be satisfied by the tensors encoding a MPS. Similar work was done in [13] for MPS with local U(1) symmetry and with open boundary conditions. We focus on translation-invariant MPS, and deal with arbitrary finite or compact Lie groups. Clearly, one could come up with arbitrarily complicated constructions of states with a local symmetry (e.g. by using many kinds of symmetric tensors). Our analysis is therefore limited to three physically meaningful settings corresponding to: states describing matter, pure gauge field states and states of both matter and gauge field. In our analysis the matter degrees of freedom are represented by "spins"; this could in principle be extended to fermionic systems, and in particular to Majorana fermions.

For states describing only matter we find that local symmetries can only be trivial, and show how to gauge such states by adding another degree of freedom. When investigating pure gauge states we show that local symmetry in MPS requires a specific structure of the Hilbert space describing the gauge field degree of freedom. In Wilson's lattice gauge theories, in order to obtain minimal coupling in a continuum limit, the gauge field degree of freedom is set as a group element in the same

representation as the one acting on the matter [3]. In the Hamiltonian formulation, the corresponding Hilbert space is isomorphic to $L^2(G)$, equipped with the left and right regular representations [36], and is referred to by Kogut and Susskind as "the rigid rotator" (in the $SU(2)$ case) [5]. The structure that we find for the gauge field Hilbert space is more general and contains the rotator-like space introduced by Kogut and Susskind as a particular case.

In the matter and gauge field setting we show that, similar to the case of MPS with a global symmetry, the tensor describing the matter degree of freedom is a (generalized) vector operator, and its structure is therefore determined by the Wigner–Eckart theorem; the gauge field tensor's structure is simpler: it is an intertwining map that translates the physical symmetry operators into a group action on the virtual (bond) spaces. This is a one dimensional version of the construction principle used in [34] - our work describes the sense in which this construction method is unique and the available structural and parametric freedom in choosing the tensors. However, the structure we derive allows for more general gauge invariant MPS, namely, ones that do not arise as a result of gauging a global symmetry or coupling matter to a pure gauge field. We construct examples of such states: while possessing a local symmetry when coupled to each other, the matter and gauge field degrees of freedom do not retain their individual symmetries when separated. Finally, we discuss mutual implications between the condition of local symmetry of the pure gauge field and the condition of global symmetry of the matter when the two can be coupled to each other to produce a MPS with local symmetry.

The paper is organized as follows. In Section 2 we introduce the basic notation and define the settings which will be investigated in subsequent sections. Section 3 presents a summary of our results. In Section 4 we review the known classification of MPV with a global symmetry. In Section 5 we derive the proofs of the stated results.

2. Formalism

In this section we introduce the MPS formalism and the notation used in this paper. We present the different settings of states and symmetries that will be the focus of investigation in subsequent sections. We motivate the choices of those settings, and relate them to physical theories. This section covers all the definitions and the essential background needed in order for our results to be stated in Section 3.

2.1. Matrix product vectors

We consider matrix product vectors (MPV) rather than states (MPS). The distinction is emphasized because MPV can refer to unnormalized MPS as well as to matrix product operators, to which our results can also be applied. Moreover, in the following we shall define symmetries in terms of equalities between vectors and not states, i.e. we shall not allow a phase difference. For a comprehensive introduction to MPS we refer the reader to [9,37,38]. In the following we shall review the basic definitions, and quote essential results.

Let $\mathcal{H}$ be a d-dimensional Hilbert space. A matrix product vector (MPV) is a vector $|\psi_A^N\rangle \in \mathcal{H}^{\otimes N}$ given by

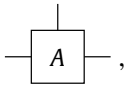
$$|\psi_A^N\rangle = \sum_{\{i\}} \mathrm{Tr}\left(A^{i_1}A^{i_2}\dots A^{i_N}\right)|i_1 i_2 \dots i_N\rangle\,, \tag{1}$$

where $\{A^i | i = 1,\dots,d\}$ are $D \times D$ matrices and $\{|i\rangle | i = 1,\dots,d\}$ is an orthonormal basis in $\mathcal{H}$. The dimension of the matrices - D - is called the bond dimension of A. We say that the tensor A, which consists of the matrices A^i, generates the MPV $|\psi_A^N\rangle$; in fact, it generates a family of vectors: $\left\{|\psi_A^N\rangle | N \in \mathbb{N}\right\}$. We refer to the entire family of vectors as the MPV generated by A.

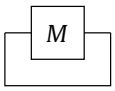
A MPV of this form is translationally invariant (TI). It is possible to describe vectors that are not TI in a similar way, with a different tensor associated with each tensor copy of $\mathcal{H}$. Throughout this paper we consider only TI-MPV.

In order to avoid cumbersome notation involving many indices, we will use the graphical notation commonly used in tensor networks. Each tensor is denoted by a rectangle with lines connected to it.

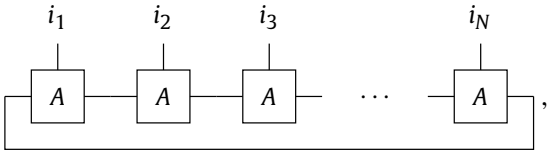
Each line corresponds to an index of the tensor. For example, the tensor A generating the MPV above is represented as:



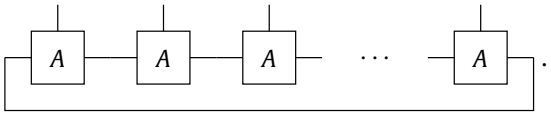
where the top line corresponds to the physical index: $i = 1, \ldots, d$, and the horizontal lines — to the ("virtual" or "bond") matrix indices: $\alpha = 1, \ldots, D$. Contraction of tensor indices is indicated by connecting the respective lines. If M is a square matrix, i.e. a rank 2 tensor, then $\mathrm{Tr}(M)$ is denoted by:



The coefficient corresponding to the $|i_1 i_2 \ldots i_N\rangle$ basis element of the MPV $|\psi_A^N\rangle$ in Eq. (1) is denoted by:



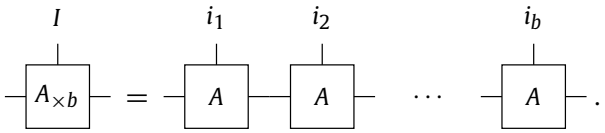
where we specified the values of the physical indices. We identify the MPV of length N generated by A with the set of its coefficients and denote the MPV as:



Definition 2.1. Let A be a tensor composed of matrices $\{A^i\}$. Blocking of b copies of A defines a new tensor denoted by $A_{\times b}$, which is composed of the matrices given by the b-fold products of A^i, and are numbered by an index $I := (i_1, i_2, \ldots, i_b)$:

$$\left\{(A_{\times b})^I = A^{i_1} A^{i_2} \ldots A^{i_b} \mid \; i_1, i_2, \ldots, i_b = 1, \ldots, d_A\right\} .$$

The new index I corresponds to the basis $\{|I\rangle := |i_1\rangle \otimes |i_2\rangle \otimes, \ldots, \otimes |i_b\rangle\}$ of $\mathcal{H}^{\otimes b}$. Graphically:



The MPV of length N generated by $A_{\times b}$ is $|\psi_{A_{\times b}}^N\rangle \in \left(\mathcal{H}^{\otimes b}\right)^{\otimes N}$.

Definition 2.2 (*Injective Tensor*)**.** A tensor A consisting of $D \times D$ matrices $\{A^i\}_{i=1}^d$ is injective if

$$span\left\{A^i \mid i = 1, \ldots, d\right\} = \mathcal{M}_{D\times D} ,$$

where $\mathcal{M}_{D\times D}$ is the algebra of $D \times D$ matrices.

Definition 2.3. Let A be a tensor consisting of matrices $\{A^i\}_{i=1}^d$. The completely positive (CP) map associated with A is defined by:

$$E_A(\cdot) = \sum_{i=1}^{D} A^i \cdot A^{i^\dagger} ,$$

i.e., the matrices $\{A^i\}$ are the Kraus operators of E_A [39].

Definition 2.4 (*Normal Tensor*)**.** a tensor A, consisting of $D\times D$ matrices $\{A^i\}_{i=1}^d$, is normal if there exists $L\in\mathbb{N}$ such that:

$$span\left\{A^{i_1}A^{i_2}\dots A^{i_L}\mid i_1,i_2,\dots,i_L=1,\dots,d\right\}=\mathcal{M}_{D\times D}\,,$$

where $\mathcal{M}_{D\times D}$ is the algebra of $D\times D$ matrices. That is, A is normal if it becomes injective after blocking a sufficient number of its copies. In addition we require that the spectral radius of the CP map E_A is equal to 1.

Remark 2.1. If a tensor becomes injective after blocking L_0 copies, it is also injective when blocking any number $L\geq L_0$ of copies. There is an upper bound on the minimal number of copies of a normal tensor needed to be blocked in order for the blocked tensor to be injective, which depends only on its bond dimension [40].

Proposition 2.1. *A tensor is normal (Definition 2.4) iff the CP map associated with it is primitive (irreducible and non-periodic)* [39].

Definition 2.5 (*Canonical Form*)**.** A tensor A is in CF if the matrices A^i are block diagonal and have the following structure:

$$A^i=\oplus_{k=1}^n \nu_k A_k^i\,, \tag{2}$$

where $\{A_k\}$ are normal tensors and ν_k are constants.

Definition 2.6 (*Canonical Form II*)**.** A is in CFII if in addition to being in CF, for any k appearing in Eq. (2) the CP map E_{A_k} is trace preserving, and has a positive full rank diagonal fixed point $\Lambda_k>0$.

Proposition 2.2. *Let $|\psi_A^N\rangle$ be the MPV generated by a tensor A. If the CP map E_A has no periodic irreducible blocks, then there exists a tensor $\tilde{A}$ in CF (or CFII) such that:*

$$|\psi_A^N\rangle=|\psi_{\tilde{A}}^N\rangle\,,\forall N\in\mathbb{N}\,.$$

If E_A does have periodic blocks, then there exist a tensor $\tilde{A}$ in CF (of CFII) and $b\in\mathbb{N}$ such that:

$$|\psi_{A_{\times b}}^N\rangle=|\psi_{\tilde{A}}^N\rangle\,,\forall N\in\mathbb{N}\,,$$

where $A^{\times b}$ is the tensor obtained by blocking b copies of A (Definition 2.1) [38].

Definition 2.7 (*Basis of Normal Tensors*)**.** Let A be a tensor in CF. A set of tensors $\{\hat{A}_j\}$ is said to be a basis of normal tensors (BNT) of A if $\hat{A}_j$ are normal tensors, and for every A_k appearing in A's expansion (Eq. (2)) there exists a unique $\hat{A}_j$, an invertible matrix V and a phase $e^{i\phi}$ such that $A_k=e^{i\phi}V^{-1}\hat{A}_jV$.

From now on whenever we consider a tensor A in CF we shall write it in terms of a BNT $\{A_j\}_{j=1}^m$:

$$A^i=\oplus_{j=1}^m\oplus_{q=1}^{r_j}\mu_{j,q}V_{j,q}^{-1}A_j^iV_{j,q}\,. \tag{3}$$

The MPV of length N generated by such a tensor A takes the form:

$$|\psi_A^N\rangle=\sum_{j=1}^m\sum_{q=1}^{r_j}\left(\mu_{j,q}\right)^N|\psi_{A_j}^N\rangle\,.$$

2.2. Representation theory

In this section we introduce projective representations. We review basic facts from representation theory, stated in the more general setting of projective representation, following [41,42]. Next, we describe how the general setting of a MPV with a symmetry with respect to a finite dimensional representation $\Theta(g)$, can be simplified by writing the MPV in a form compatible with the decomposition of $\Theta(g)$ into irreducible representations. Finally, we quote two theorems: Schur's lemma and the Wigner–Eckart theorem, that will allow us to classify the tensors generating symmetric MPVs.

2.2.1. Projective representations

Let $\mathcal{H}$ be a finite dimensional Hilbert space. Denote by $\mathrm{U}(\mathcal{H})$ the group of unitary operators on $\mathcal{H}$. Throughout the paper, unless explicitly stated otherwise, G will always refer to a finite group or a compact Lie group.

Definition 2.8. A function $\gamma : G \times G \to U(1)$ satisfying:

$$\gamma(g,h)\gamma(gh,f) = \gamma(g,hf)\gamma(h,f), \quad \forall g,h,f \in G$$
$$\gamma(g,e) = \gamma(e,g) = 1, \quad \forall g \in G\,,$$

where $e \in G$ is the trivial element, is called a multiplier of G. For compact Lie groups we require γ to be continuous.

Definition 2.9. A projective unitary representation of a group G on $\mathcal{H}$ is a map $\Theta : G \to \mathrm{U}(\mathcal{H})$ such that for all $g, h \in G$ $\Theta(g)\Theta(h) = \gamma(g,h)\Theta(gh)$, where γ is a multiplier of G.

That is, projective unitary representations are unitary representations up to a phase factor. Throughout this paper all representations will be assumed to be unitary and finite dimensional. From this point on, *unitary representation* shall be used to emphasize that it is not projective. *Projective representations* can refer to both, as unitary representations are a particular case of projective representations, namely, they are the ones with the trivial multiplier.

Two projective representations $(\Theta, \mathcal{H})$ and $(\Theta', \mathcal{H}')$ with multipliers γ and γ' are *equivalent in the sense of projective representations* if there exist an isomorphism $\phi : \mathcal{H} \to \mathcal{H}'$ and a function $\mu : G \to U(1)$ such that $\Theta'(g)\phi = \mu(g)\phi\Theta(g)$ for all $g \in G$. Their multipliers then satisfy:

$$\gamma'(g,h) = \gamma(g,h)\mu(g)\mu(h)\mu(gh)^{-1}\,. \tag{4}$$

Eq. (4) defines an equivalence relation on the group of multipliers of G. The quotient of the subgroup of multipliers of the form $\gamma(g,h) = \mu(g)\mu(h)\mu(gh)^{-1}$ in the group of all multipliers is the second cohomology group $H^2(G, U(1))$ of G over $U(1)$ [42]. When two projective representations Θ and Θ' have multipliers related by Eq. (4), for some function $\mu : G \to U(1)$ we say they are in the same cohomology class.

Definition 2.10. Two projective representations $(\Theta, \mathcal{H})$ and $(\Theta', \mathcal{H}')$ with the same multiplier γ are *equivalent* if there exists an isomorphism $\phi : \mathcal{H} \to \mathcal{H}'$ such that $\Theta'(g)\phi = \phi\Theta(g)$ for all $g \in G$. We denote $\Theta'(g) \cong \Theta(g)$.

2.2.2. Complete reducibility

Fix a choice of representatives from the equivalence classes (Definition 2.10) of irreducible projective representations of G with multiplier γ; denote them by $D^j_\gamma : G \to \mathrm{U}(\mathcal{H}_j)$. Fixing a basis $\{|i\rangle\}$ in $\mathcal{H}_j$ for every j defines the irreducible projective representation matrices: $D^j_\gamma(g) = \sum_{m,n} D^j_\gamma(g)_{m,n}|m\rangle\langle n|$. These generalize the $SU(2)$ Wigner matrices to projective representations of arbitrary groups.

Let $\mathcal{H}$ be a finite dimensional Hilbert space, and let $\Theta : g \mapsto \Theta(g)$ be a projective representation of G with multiplier γ. For finite and compact groups any finite dimensional projective representation is fully reducible and is equivalent to a direct sum of irreducible projective representations $\oplus_j D^j_\gamma(g)$ with the same multiplier, i.e., there exists a basis $\{|j,m\rangle\}$ of $\mathcal{H}$ such that:

$$\Theta(g)|j,m\rangle = \sum_n D^j_\gamma(g)_{n,m}|j,n\rangle\,. \tag{5}$$

We refer to such a basis as the irreducible representation basis of $\Theta(g)$ (in general it is not unique, e.g., when an irreducible representation appears multiple times [43]; we shall assume a choice of such a basis).

When considering a representation acting on a MPV, it is convenient to write the MPV in the irreducible representation basis. In the following we describe how this is achieved, and show that it does not interfere with CF properties of the tensor generating the MPV.

Remark 2.2. A change of basis of the physical space from $\{|i\rangle\}$ to the irreducible representation basis $\{|j, m\rangle\}$ (Eq. (5)), involves a transformation of the tensor generating the MPV: $A \mapsto \tilde{A}$, where $\tilde{A}$ consists of the matrices $\{\tilde{A}^{j,m} = \sum_i \langle j, m \mid i\rangle A^i\}$. This is easily seen by inserting an identity operator $\sum_{j,m} |j, m\rangle\langle j, m|$ for every copy of $\mathcal{H}$ in the definition of $|\psi_A^N\rangle$ (Eq. (1)).

Proposition 2.3. *Let $\{A^i\}_{i=1}^d$ be the Kraus operators defining a CP map E_A. For any unitary $d \times d$ matrix U the matrices $\{\sum_j U_{i,j} A^j\}_{i=1}^d$ define the same CP map* [39].

Corollary 2.1. *Let A be a tensor in CF (CFII) composed of the matrices $\{A^i\}$ corresponding to the basis $\{|i\rangle\}$ of $\mathcal{H}$. Then the tensor $\tilde{A}$, composed of the matrices $\{\tilde{A}^{j,m} = \sum_i A^i \langle j, m \mid i\rangle\}$ as in Remark 2.2, is also in CF (CFII).*

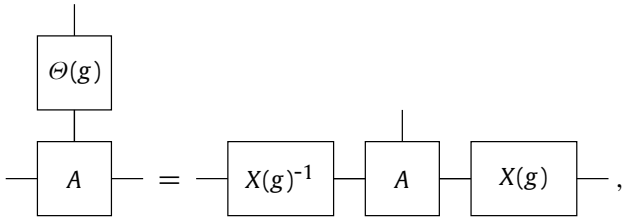
Proof. $\tilde{A}$ has the same block structure as A (Eq. (2)):

$$\tilde{A}^{j,m} = \oplus_{k=1}^n \nu_k \tilde{A}_k^{j,m} = \oplus_{k=1}^n \nu_k \sum_i \langle j, m \mid i\rangle A_k^i \,.$$

According to Proposition 2.1, the normality and CFII properties of each block $\tilde{A}_k$ are defined by the CP map associated to it. Proposition 2.3 says this maps is not affected by the transformation $A_k \mapsto \tilde{A}_k$ because $\{\langle j, m \mid i\rangle\}$ are the entries of a unitary matrix. Each block $\tilde{A}_k$ is therefore a normal tensor (and in CFII). □

2.2.3. Intertwining relations

It was shown in [44,45] that an injective tensor A which generates a MPV with a global symmetry with respect to a representation Θ_g, satisfies:



(6)

i.e., for all $i = 1, \ldots, d$: $\sum_{i'} \Theta(g)_{ii'} A^{i'} = X(g)^{-1} A^i X(g)$, where $X(g)$ is a projective representation of G. While we will make the precise statement and derive this result later, we now point out that in Eq. (6) the tensor A translates the action of $\Theta(g)$ on the physical space into a group action on the virtual space.

In the following, we quote two theorems: Schur's lemma and the Wigner–Eckart theorem, which can be used to classify tensors satisfying such intertwining relations.

Definition 2.11 (*Intertwining Map*)**.** Let (η, V) and (π, W) be projective representations of a group G with the same multiplier. A linear map $T : V \to W$ is called an intertwining map if $\pi(g)T = T\eta(g), \quad \forall g \in G$.

Lemma 2.1 (*Schur's Lemma*)**.** *An intertwining map between irreducible projective representations with the same multiplier is zero if they are inequivalent, and proportional to the identity if they are equal* [42].

The tensor product of two irreducible projective representations with multipliers γ and γ' is a projective representation with multiplier $\gamma\gamma'$ ($\gamma\gamma' : (g, h) \mapsto \gamma(g, h)\gamma'(g, h)$), and is generally a reducible one. The unitary map that realizes the decomposition of $D^j_\gamma(g) \otimes D^l_{\gamma'}(g)$ into a direct sum of irreducible representations $\oplus_{J\in\mathfrak{J}} D^J_{\gamma\gamma'}$ is the Clebsch–Gordan map whose matrix elements are the Clebsch–Gordan coefficients $\langle j, m; l, n \mid J, M\rangle$, which are determined by the choice of the representation matrices D^j_γ (for a discussion of their uniqueness having fixed the representation matrices see [43]).

The following is a generalization of the $SO(3)$ vector operators, well known in quantum mechanics [41].

Definition 2.12 (*Vector Operator*)**.** Let $(\eta, V), (\pi, W)$ and $(\kappa, \mathcal{H})$ be projective representations of G with $dim(\mathcal{H}) = d$. A vector operator with respect to (κ, π, η) is a d-tuple of linear operators $\vec{A} = (A^1, A^2, \ldots, A^d), A^i : V \mapsto W$ which, for all $g \in G$ and all $\vec{v} \in \mathcal{H}$, satisfies:

$$(\kappa(g)\vec{v}) \cdot \vec{A} = \pi(g) \left(\vec{v} \cdot \vec{A}\right) \eta(g)^{-1} \tag{7}$$

where $\vec{v} \cdot \vec{A} := \sum_i v^i A^i$.

It was shown in [44] that Eq. (6) can be used to determine the tensor A satisfying it, and that it consists of Clebsch–Gordan coefficients. We will derive the same result using a generalized version of the well known Wigner–Eckart theorem, using the fact that Eq. (6) resembles a vector operator relation for A (Definition 2.12).

Theorem 2.1 (*Wigner–Eckart*)**.** *Let $D^{J_0}_{\gamma}(g)$, $D^{j}_{\gamma'}(g)$ and $D^{l}_{\gamma''}(g)$ be irreducible projective representations. Let $\vec{A}$ be a vector operator with respect to $(\kappa := D^{J_0}_{\gamma}, \pi := D^{j}_{\gamma'}, \eta := D^{l}_{\gamma''})$. If $\gamma\gamma'' \neq \gamma'$, then $A = 0$. Otherwise (if $\gamma\gamma'' = \gamma'$), then $\{A^M | M = 1, \ldots, dim(J_0)\}$ are of the form:*

$$A^M = \sum_{J \in \mathfrak{J}: D^J = D^{J_0}} \alpha_J \sum_{m,n} \left\langle j, m; \bar{l}, n \mid J, M \right\rangle |m\rangle\langle n| \,, \tag{8}$$

where $\mathfrak{J}$ is the set of irreducible projective representation indices appearing in the decomposition of $D^{j}_{\gamma'}(g) \otimes \overline{D^{l}_{\gamma''}(g)}$, $\left\langle j, m; \bar{l}, n \mid J, M \right\rangle$ are the Clebsch–Gordan coefficients of this decomposition, $\overline{D^{l}_{\gamma''}(g)}$ is the complex conjugate representation to $D^{l}_{\gamma''}(g)$, $\{|m\rangle\}$ and $\{|n\rangle\}$ are the irreducible representation bases: $\pi(g)|m\rangle = \sum_{m'} D^{j}_{\gamma'}(g)_{m',m}|m'\rangle$, $\eta(g)|n\rangle = \sum_{n'} D^{l}_{\gamma''}(g)_{n',n}|n'\rangle$ and α_J are arbitrary constants.

For a proof of the theorem in the familiar $SO(3)$ setting, we refer the reader to [41]; for a proof in the setting of projective representations see [46].

Remark 2.3. Apart from the freedom of choosing the constants $\{\alpha_J\}$ in Eq. (8), there is an additional freedom which comes from the fact that the Clebsch–Gordan coefficients are not uniquely determined by the irreducible representation matrices [43].

Remark 2.4. The multiplier of the complex conjugate projective representation $\overline{D^{l}_{\gamma}(g)}$ is γ^{-1}. We will always use Theorem 2.1 with $\gamma \equiv 1$, then $A = 0$ unless $\gamma' = \gamma''$.

Remark 2.5. We assume a choice of a unique representative in each equivalence class of irreducible projective representations of G, so any two are either inequivalent or are represented by the same matrices.

Remark 2.6. A is zero if $D^{J_0}_{\gamma}(g)$ does not appear in the decomposition of $D^{j}_{\gamma'}(g) \otimes \overline{D^{l}_{\gamma''}(g)}$. There is a J summation in Eq. (8) because in general the same irreducible representation could appear multiple times in the decomposition of the tensor product of two irreducible representations.

2.3. Physical states and their symmetries

Gauge theories involve the dynamics of two kinds of degrees of freedom: *matter* and *gauge field*. Given those two ingredients, one can consider three types of states: states of only matter degrees of freedom, states of only gauge field degrees of freedom and states of both matter and gauge field. These correspond to non-interacting theories, pure gauge theories and interacting gauge theories respectively (where interactions are understood as those between matter and gauge degrees of freedom).

When constructing a gauge theory one usually starts from an interaction-free theory of the matter degree of freedom which is invariant with respect to a group of global transformations, i.e., the same

group element acting in each point in space (or space–time). Adding an additional degree of freedom – the gauge field – with its own transformation law with respect to the group, allows to define local symmetry operators which act on both the matter and the gauge field degrees of freedom. These operators commute with the transformed (gauged) Hamiltonian, and the subspace of states which is invariant under all such operators is considered as the space of physical states. The generators of such local symmetry operators are the so-called Gauss law operators. They correspond to locally conserved quantities (charges), i.e., associated to each point in space (or space–time).

Conversely, one could start from a pure gauge field theory with a local symmetry and couple a matter degree of freedom to it, once again resulting in a system with local symmetry. Finally one could have matter and gauge field coupled in such a way that the combined state has a local symmetry but neither the mass state nor the gauge field state have a symmetry on their own.

We shall now describe the three types of MPVs considered in this paper, corresponding to the above mentioned types of states, and for each one of them define the symmetries which will be investigated in subsequent sections.

2.3.1. Matter MPV

Let $\mathcal{H}_A$ be a d_A dimensional Hilbert space corresponding to a single degree of freedom ("spin"). Consider N such "spins" positioned on a one dimensional lattice, with periodic boundary conditions. A tensor A consisting of square matrices $\{A^i\}_{i=1}^{d_A}$ generates a TI-MPV that describes a state of the chain of matter "spins". Let Θ be a unitary representation of G on $\mathcal{H}_A$, $\Theta : g \mapsto \Theta(g)$.

It is well known that in order to lift a global symmetry to be a local one, an additional degree of freedom must be introduced [1]. When investigating the possibility of a local symmetry for a matter MPV, we find this statement reaffirmed (see Theorem 1). We define the setting of the theorem in the following:

Definition 1 (*Local Symmetry for Matter MPV*)**.** A MPV $|\psi_A^N\rangle$ has a local symmetry with respect to $\Theta(g)$ if for all $N \in \mathbb{N}$:

$$\Theta_{g_1} \otimes \Theta_{g_2} \otimes \cdots \otimes \Theta_{g_N} |\psi_A^N\rangle = |\psi_A^N\rangle, \quad \forall g_1, g_2, \ldots, g_N \in G\,.$$

Global symmetry in MPS have been studied extensively [44,47]. In order for this paper to be self contained, we quote and then derive the main result, which classifies the tenors A that generate MPV with the following symmetry:

Definition 2 (*Global Symmetry for Matter MPV*)**.** A MPV $|\psi_A^N\rangle$ has a global symmetry with respect to $\Theta(g)$ if for all $N \in \mathbb{N}$:

$$\Theta_g \otimes \Theta_g \otimes \cdots \otimes \Theta_g |\psi_A^N\rangle = |\psi_A^N\rangle, \quad \forall g \in G\,.$$

Remark 2.7. The condition of a local symmetry (Definition 1) is equivalent to invariance under any single-site group action (all $g_i = e$ except one). For TI-MPV it is therefore sufficient to consider only $g_1 \neq e$.

2.3.2. Gauge field MPV

Next we shall consider a case in which the local transformations act on two neighboring sites of a TI-MPV, which will be eventually seen as the pure gauge case.

Let $\mathcal{H}_B$ be a d_B dimensional Hilbert space corresponding to a single "spin". Consider N such spins positioned on a one dimensional lattice, with periodic boundary conditions. A tensor B consisting of square matrices $\{B^i\}_{i=1}^{d_B}$ generates a TI-MPV that describes a state of the chain of gauge field "spins".

Definition 3 (*Local Symmetry for Gauge Field MPV*)**.** Let $\mathcal{R}$, $\mathcal{L}$ be two projective representations of G on $\mathcal{H}_B$, $\mathcal{R} : g \mapsto \mathcal{R}(g)$, $\mathcal{L} : g \mapsto \mathcal{L}(g)$ with multipliers γ and γ^{-1}, so that the tensor product $\mathcal{R}(g) \otimes \mathcal{L}(g)$ is a unitary representation. A MPV $|\psi_B^N\rangle$ has a local symmetry with respect to $\mathcal{R}(g) \otimes \mathcal{L}(g)$ if for all $N \in \mathbb{N}$ and for any two neighboring lattice sites K and $K+1$:

$$\mathcal{R}_g^{[K]} \otimes \mathcal{L}_g^{[K+1]} |\psi_B^N\rangle = |\psi_B^N\rangle, \quad \forall g \in G\,.$$

2.3.3. Matter and gauge field MPV

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be as in Sections 2.3.1 and 2.3.2 respectively. Consider a lattice of length $2N$ with matter and gauge field spins alternating among sites. Tensors A and B, consisting of $D_1 \times D_2$ matrices $\{A^i\}_{i=1}^{d_A}$ and $D_2 \times D_1$ matrices $\{B^j\}_{j=1}^{d_B}$ respectively, generate a TI-MPV (in the sense of translating two sites) that describes a state of the chain of matter and gauge field "spins". The MPV, generated by a tensor we denote AB, takes the form:

$$|\psi_{AB}^N\rangle = \sum_{\{i\},\{j\}} \mathrm{Tr}\left(A^{i_1}B^{j_1}A^{i_2}B^{j_2}\ldots A^{i_N}B^{j_N}\right)|i_1j_1i_2j_2\ldots i_Nj_N\rangle\ .$$

In lattice gauge theories, the matter degrees of freedom are located on the sites of a lattice whereas the gauge field degrees of freedom — on the links connecting adjacent sites [3]. In the one dimensional case, our setting differs from this structure only in notation, e.g., we could have chosen to call the even numbered sites "links".

Let $\Theta(g)$ and $\mathcal{R}(g)$, $\mathcal{L}(g)$ be as in Sections 2.3.1 and 2.3.2 respectively.

Definition 4 (*Local Symmetry for Both Matter and Gauge Field MPV*)**.** A MPV $|\psi_{AB}^N\rangle$ has a local symmetry with respect to $\mathcal{R}(g)\otimes\Theta(g)\otimes\mathcal{L}(g)$ if for all $N \in \mathbb{N}$ and for any three neighboring lattice sites numbered $2K$, $2K+1$ and $2K+2$ (corresponding to $\mathcal{H}_B \otimes \mathcal{H}_A \otimes \mathcal{H}_B$):

$$\mathcal{R}(g)^{[2K]} \otimes \Theta(g)^{[2K+1]} \otimes \mathcal{L}(g)^{[2K+2]}|\psi_{AB}^N\rangle = |\psi_{AB}^N\rangle, \quad \forall g \in G\ .$$

2.4. Generators and Gauss' law

In the previous section we defined the symmetries in terms of representations of a group G. For matrix Lie groups it is often the case that one could describe the same symmetry in terms of representations of the Lie algebra $\mathfrak{g}$ of G. While the two descriptions are mathematically equivalent, it is precisely the elements of the Lie algebra representation that correspond to observables in physical theories. Such observables are conserved by the dynamics in a theory which respects the symmetry, and are therefore of great importance.

To each scenario described above (Sections 2.3.1–2.3.3) correspond different such observables, and physical theories corresponding to the different settings – matter, gauge field or matter and gauge field – observe different conservation laws. In the following we describe the relation of those settings to physical lattice gauge theories [36].

When G is a compact and connected Lie group, e.g. $U(1)$ or $SU(N)$, the exponential map $\exp : \mathfrak{g} \to G$ is surjective. Thus every group element can be written as an exponential of an element in the Lie algebra $\mathfrak{g}$ [48]. Let $\mathcal{R}(g)$, $\mathcal{L}(g)$ and $\Theta(g)$ be representations on $\mathcal{H}_B$ and $\mathcal{H}_A$ respectively (for $SU(N)$ we can always choose $\mathcal{R}(g)$ and $\mathcal{L}(g)$ to be unitary representations keeping $\mathcal{R}(g)\otimes\mathcal{L}(g)$ unchanged [41]), and let $|\psi_{AB}^N\rangle$ be as defined in Section 2.3.3. We can express the physical representations as exponentials of generators:

$$\Theta(g) = \exp\left(i\sum_a Q_a\varphi_a(g)\right)$$

$$\mathcal{R}(g) = \exp\left(i\sum_a R_a\varphi_a(g)\right)$$

$$\mathcal{L}(g) = \exp\left(i\sum_a L_a\varphi_a(g)\right)\ ,$$

where $\{\varphi_a(g)\}_{a=1}^{dim(\mathfrak{g})}$ are real parameters and $\{R_a\}_{a=1}^{dim(\mathfrak{g})}$, $\{L_a\}_{a=1}^{dim(\mathfrak{g})}$ and $\{Q_a\}_{a=1}^{dim(\mathfrak{g})}$ are Hermitian operators on $\mathcal{H}_B$ and $\mathcal{H}_A$ respectively such that $\{iR_a\}$, $\{iL_a\}$ and $\{iQ_a\}$ are bases of the respective Lie algebras. In the

Hamiltonian formulation of lattice gauge theories [5,36] $\{R_a\}$ and $\{L_a\}$ satisfy the Lie algebra relations:

$$[R_a, R_b] = if_{abc}R_c$$
$$[L_a, L_b] = if_{abc}R_c$$
$$[R_a, L_b] = 0\ ,$$

where f_{abc} are the structure constants of the Lie algebra $\mathfrak{g}$. $\{Q_a\}$ satisfy the relations:

$$[Q_a, Q_b] = if_{abc}Q_c\ .$$

The local symmetry transformations appearing in the matter and gauge field MPV scenario (Definition 4):

$$\mathcal{R}^{[2K]}(g) \otimes \Theta^{[2K+1]}(g) \otimes \mathcal{L}^{[2K+2]}(g)|\psi_{AB}^N\rangle = |\psi_{AB}^N\rangle\ , \tag{9}$$

are generated by the operators:

$$G_a^{[2K+1]} := \left(R_a^{[2K]} + Q_a^{[2K+1]} + L_a^{[2K+2]}\right)\ .$$

Differentiating Eq. (9) with respect to any of the parameters φ_a we obtain:

$$\left(R_a^{[2K]} + Q_a^{[2K+1]} + L_a^{[2K+2]}\right)|\psi_{AB}^N\rangle = G_a^{[2K+1]}|\psi_{AB}^N\rangle = 0\ . \tag{10}$$

This is the lattice version of Gauss' law. In physical theories, states $|\psi_A\rangle$ have a global symmetry generated by $\{Q_a\}$ - the $SU(N)$ charge operators. In the $U(1)$ case there is one generator Q - the electric charge operator; furthermore, for Abelian groups $L = -R$. In that case Eq. (10) says that at each lattice site corresponding to matter, the charge is equal to the difference between the values of L on the right and on the left of it (the 1D lattice divergence of L). This becomes Gauss' law when taking a continuum limit. L is therefore identified as the electric field. Analogously, in the $SU(N)$ case $\{R_a\}$ and $\{L_a\}$ are identified with right and left electric fields respectively [36].

The same kind of equation can be obtained for the case of a gauge field MPV with a local symmetry (Definition 3):

$$\left(R_a^{[K]} + L_a^{[K+1]}\right)|\psi_B^N\rangle = 0\ .$$

In the case of a global symmetry for a matter MPV, differentiating the symmetry relation (Definition 2), we obtain a global operator — the total charge:

$$\sum_K Q_a^{[K]}|\psi_A^N\rangle = 0\ .$$

3. Results

We summarize the results presented in this paper, first stating the main results of each of the cases presented above, and then turning to a more detailed and formal description. The detailed proofs will be given in the subsequent sections. For each one of the settings introduced in the previous section, we shall first show that the symmetry condition implies a transformation relation satisfied by the tensor(s) generating the MPV. Second, we shall show that those transformation relations determine the structure of the tensor(s). For each setting we shall then discuss implications of the derived tensor structures.

3.1. Matter MPV with local symmetry

We show that a MPV with one degree of freedom – the mass "spins" – can have a local symmetry as in Definition 1, only if it is the trivial one. This is consistent with the way gauge invariant states are usually constructed in lattice gauge theories, as well as with the construction of continuum gauge theories, where an additional degree of freedom is introduced. The first observation is a general one, not restricted to MPVs:

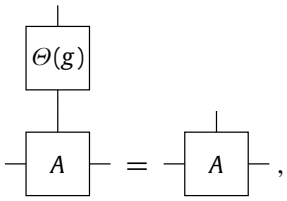
Proposition 1. *Let $\mathcal{H}$ be a finite dimensional Hilbert space and let $\Theta : g \mapsto \Theta(g)$ be a representation on $\mathcal{H}$. Let $|\psi^N\rangle \in \mathcal{H}^{\otimes N}$ be a vector with a local symmetry, i.e.*

$$\Theta(g_1) \otimes \Theta(g_2) \otimes \cdots \Theta(g_N)|\psi^N\rangle = |\psi^N\rangle, \quad \forall g_1, g_2, \ldots, g_N \in G\,.$$

Then $|\psi^N\rangle \in \mathcal{H}_0{}^{\otimes N}$, where $\mathcal{H}_0 \subset \mathcal{H}$ is the subspace on which $\Theta(g)$ acts trivially.

In the following we show that for MPVs a similar statement to Proposition 1 can be made for the tensor generating the MPV. Let $|\psi_A\rangle$ and $\Theta(g)$ be as in Section 2.3.1. According to Proposition 2.2, given an arbitrary tensor A generating $|\psi_A\rangle$, one can obtain a tensor in CF which generates the same state, (possibly after blocking A). We therefore assume A to be in CF.

Theorem 1. *Let A be a tensor in CF generating a MPV with a local symmetry with respect to a representation $\Theta(g)$ (Definition 1). Then for all $g \in G$ the tensor A satisfies:*



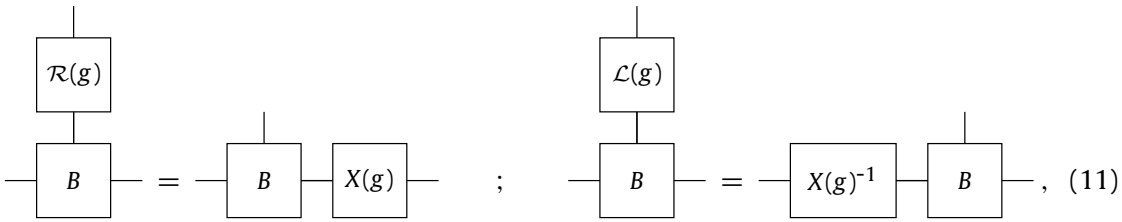
i.e., for all $i = 1, \ldots, d_A$: $\sum_{i'} \Theta(g)_{ii'} A^{i'} = A^i$.

According to Remark 2.2, the MPV generated by A can be written in terms of a tensor $\tilde{A}$, composed of the matrices $\{\tilde{A}^{j,m}\}$, corresponding to the irreducible representation basis $\{|j, m\rangle\}$ on which $\Theta(g)$ acts as $\Theta(g)|j, m\rangle = \sum_n D^j(g)_{n,m}|j, n\rangle$. According to Corollary 2.1, $\tilde{A}$ is also in CF. Applying Theorem 1 to $\tilde{A}$ leads to the following:

Corollary 1. *The matrices $\tilde{A}^{j,m}$ are non-zero only for j such that $D^j(g) \equiv \mathbb{I}_{1\times 1}$.*

3.2. Gauge field MPV

We show that a local symmetry for a gauge field MPV $|\psi_B^N\rangle$ generated by a tensor B (in CFII) (as defined in Section 2.3.2), implies the following transformation relations for B:



(11)

where $X(g)$ is a projective representation with the same multiplier as that of $\mathcal{R}(g)$. This transformation relation allows to determine the structure of the physical Hilbert space of the gauge field degree of freedom. We find that the gauge field "spins" are composed of right and left parts:

$$\mathcal{H}_B = \oplus_k \mathcal{H}_{l_k} \otimes \mathcal{H}_{r_k}\,,$$

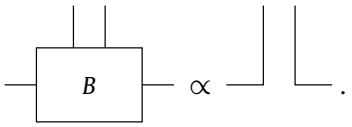
where $\mathcal{H}_{r_k}$ are irreducible representation spaces of G. The physical representations $\mathcal{R}(g)$ and $\mathcal{L}(g)$ take the forms: $\mathcal{R}(g) = \oplus_k(\mathbb{I} \otimes D^{r_k}_\gamma(g))$, $\mathcal{L}(g) = \oplus_k(D^{l_k}_{\gamma^{-1}}(g) \otimes \mathbb{I})$, and act on the right and left parts of $\mathcal{H}_B$ respectively.

The transformation relation Eq. (11) also determines the structure of the tensor B. Decompose $X(g)$ into its constituent irreducible representations and project Eq. (11) to the corresponding irreducible subspaces (virtual and physical). The obtained blocks of B intertwine irreducible representations, and their structure is therefore determined by Schur's lemma (Lemma 2.1). When the irreducible

representations in Eq. (11) match, the corresponding elementary block of B is proportional to the tensor composed of the matrices:

$$B^{m,n} = |m\rangle\langle n| \,,$$

so that B, when represented in graphical notation, takes the form:



Otherwise, if the irreducible representations do not match, that block of B is zero.

The tensor B is composed out of such elementary building blocks multiplied by constants — free parameters. Finally, we show that for any B generating a gauge field MPV with a local symmetry, one can always find a tensor A, describing a matter degree of freedom, such that the matter and gauge field MPV generated by A and B has a local symmetry.

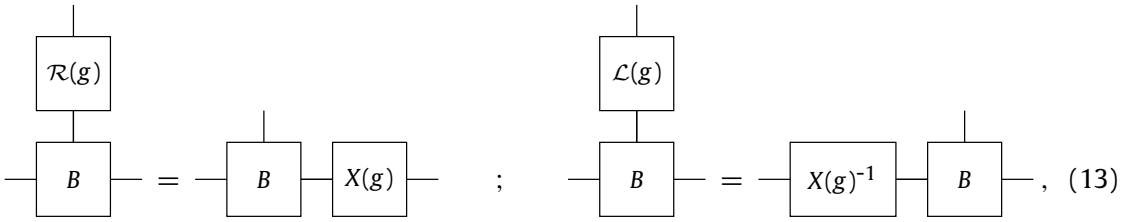
We shall now describe these results in detail, and state the relevant theorems.

Let $|\psi_B\rangle$ be a MPV generated by a tensor B and let $\mathcal{R}(g)$, $\mathcal{L}(g)$ be projective representations as defined in Section 2.3.2. As in the case of a matter MPV above, according to Proposition 2.2 we can assume B is in CFII and write it in terms of its BNT:

$$B^i = \oplus_{j=1}^{n} \oplus_{q=1}^{r_j} \mu_{j,q} B_j^i \,, \tag{12}$$

where $\{B_j\}$ are normal tensors in CFII forming a BNT of B (Definition 2.7) and $\mu_{j,q}$ are constants.

Theorem 2 (*Gauge Field MPV with a Local Symmetry*)**.** *A tensor B in CFII which generates a MPV that has a local symmetry with respect to $\mathcal{R}(g) \otimes \mathcal{L}(g)$ where $\mathcal{R}(g)$ and $\mathcal{L}(g)$ are projective representations with inverse multipliers (Definition 3), transforms under the representation matrices as:*

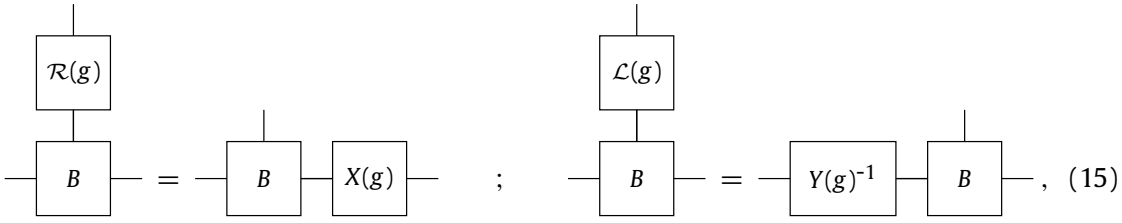


(13)

where $X(g)$ is a projective representation of G with the same multiplier as $\mathcal{R}(g)$ and with the same block structure as B (Eq. (12)):

$$X(g) = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} X_j(g) \,. \tag{14}$$

When considering matter and gauge field MPVs in the next section, we will show that in that setting, a more general relation than Eq. (13) is satisfied by the tensor B. Namely:



(15)

where $X(g)$ and $Y(g)$ are different projective representations (in the case when B is composed of non-square matrices they are of different dimensions). We shall now present results which follow from the more general relation (Eq. (15)), as they will be relevant also in the next section. Then we will apply them to the case at hand — Eq. (13) (i.e., when $X(g) = Y(g)$ and B is composed out of square matrices).

Eq. (15) allows us to determine the structure of the Hilbert space of the gauge field degree of freedom. The fact that the action of $\mathcal{R}(g)$ is translated to a matrix multiplication from the right, and

that of $\mathcal{L}(g)$ - to multiplication from the left implies that their actions on the "spin" representing the gauge field are independent, consequently the "spin" must be composed of right and left parts:

Proposition 2 (*Structure of $\mathcal{H}_B$*)**.** *Given a tensor B, projective representations $\mathcal{R}(g)$, $\mathcal{L}(g)$ with inverse multipliers γ and γ^{-1} (as defined in Section 2.3.2) and matrices $X(g)$ and $Y(g)$ which satisfy Eq. (15), the Hilbert space $\mathcal{H}_B$ can be restricted to a representation space of $G \times G$ and thus decomposes into a direct sum of tensor products of irreducible representation spaces of G:*

$$\mathcal{H}_B = \bigoplus_{k=1}^{M} \mathcal{H}_{l_k} \otimes \mathcal{H}_{r_k} ,$$

where r_k and l_k are irreducible representation labels.

The structure of $\mathcal{H}_B$ described in [34] is a particular case of this Hilbert space. There:

$$\mathcal{H}_B = \bigoplus_{k=1}^{M} \mathcal{H}_{\overline{r_k}} \otimes \mathcal{H}_{r_k} , \tag{16}$$

where $\overline{r_k}$ indicates the complex conjugate representation to r_k. Eq. (16) is a truncated version of the K–S Hilbert space, which allows to regain the whole space if M is increased such that all the irreducible representations are included. Each k sector in Eq. (16): $\mathcal{H}_{\overline{r_k}} \otimes \mathcal{H}_{r_k}$ is isomorphic to the function space spanned by

$$\left\{ D^{r_k}_{m,n} : g \mapsto D^{r_k}_{m,n}(g) \mid m, n = 1, \ldots, dim(r_k) \right\} \subset L^2(G) ,$$

with $\mathcal{R}(g)$ and $\mathcal{L}(g)$ equivalent to the right and left translations [49].

Remark 3.1. The group transformations $\mathcal{R}(g)$ and $\mathcal{L}(g)$ are equivalent, according to Proposition 2, to $\oplus_k(\mathbb{I} \otimes D^{r_k}_{\gamma}(g))$ and $\oplus_k(D^{l_k}_{\gamma^{-1}}(g) \otimes \mathbb{I})$ respectively, where $D^{i}_{\gamma}(g)$ are irreducible projective representations. Changing the basis of the physical Hilbert space (as in Remark 2.2) to $\{|l_k, m\rangle \otimes |r_k, n\rangle\}$ in which the representations take this block diagonal form, involves transforming B into $\tilde{B}$ given by the matrices: $\tilde{B}^{k,m,n} = \sum_i B^i \langle l_k, m; r_k, n \mid i\rangle$. According to Corollary 2.1 $\tilde{B}$ is also in CFII. Eq. (15) holds for the new tensor under the action of the transformed operators: $\tilde{\mathcal{R}}(g) = \oplus_k(\mathbb{I} \otimes D^{r_k}_{\gamma}(g))$ and $\tilde{\mathcal{L}}(g) = \oplus_k(D^{l_k}_{\gamma^{-1}}(g) \otimes \mathbb{I})$. We shall always assume B, $\mathcal{L}(g)$ and $\mathcal{R}(g)$ are in these forms.

Remark 3.2. The simplest case of Eq. (15) one could consider is when $\mathcal{R}(g) = \mathbb{I} \otimes D^{r}(g)$ and $\mathcal{L}(g) = D^{l}(g) \otimes \mathbb{I}$, for irreducible projective representations $D^{r}_{\gamma}(g)$ and $D^{l}_{\gamma^{-1}}(g)$. To these corresponds the basis $\{|m\rangle \otimes |n\rangle \mid m = 1, \ldots, dim(l), n = 1, \ldots, dim(r)\}$, and the matrices composing the tensor B are numbered by two indices:

$$B^{m,n} = \sum_{\alpha,\beta} B^{m,n}_{\alpha,\beta} |\alpha\rangle\langle\beta| .$$

B transforms under $\mathcal{R}(g)$ and $\mathcal{L}(g)$ in the following manner:

$$\mathcal{R}(g) : B^{m,n} \mapsto \sum_{n'} D^{r}_{\gamma}(g)_{n,n'} B^{m,n'} = B^{m,n} X(g)$$

$$\mathcal{L}(g) : B^{m,n} \mapsto \sum_{m'} D^{l}_{\gamma^{-1}}(g)_{m,m'} B^{m',n} = Y(g)^{-1} B^{m,n} .$$

We have seen in Remark 2.2 how to change the basis of the physical Hilbert space in order to bring the physical representations to block diagonal form. We would like to do the same for the virtual projective representation $X(g)$ appearing in Eq. (13). This can be achieved by a different transformation of the tensor B described in the following:

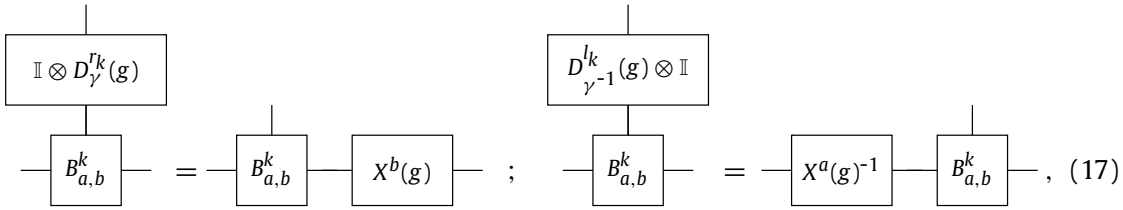
Remark 3.3. Given B, $\mathcal{R}(g)$, $\mathcal{L}(g)$ and $X(g)$ that satisfy Eq. (13), redefine B:

$$B^{k;m,n} \mapsto \tilde{B}^{k;m,n} = V^{-1} B^{k;m,n} V \ ,$$

with any invertible matrix V. The new tensor $\tilde{B}$ generates the same MPV and transform as in Eq. (13) with $X(g)$ replaced by $\tilde{X}(g) = V^{-1} X(g) V$.

Remark 3.4. Note that the transformation described in Remark 3.3 may ruin the CF property of B, as V does not in general preserve B's block structure (Eq. (12)). We shall therefore take care to use this freedom of choosing the basis of $X(g)$ only when we no longer intend to use the CF property.

Remark 3.3 allows us to assume without loss of generality $X(g)$ takes the form $\oplus_a X^a(g)$, where $X^a(g)$ are irreducible projective representations. Next we project Eq. (13) to the k sector of the physical Hilbert space (Remark 3.1) and to the (a, b) block in the virtual space, since the representations are block diagonal they commute with the projection operators for every group element $g \in G$. We therefore obtain:



(17)

where $B^k_{a,b}$ is the tensor that consists of the (a, b) blocks of the matrices $B^{k;m,n}$.

The reduction procedure described above motivates the following definition of an elementary B block. Next we shall show that the irreducible representations appearing in Eq. (17) determine such blocks up to a constant.

Definition 3.1. An elementary block of the tensor B is one which satisfies Eq. (15), where $\mathcal{R}(g) = \mathbb{I} \otimes D^r_{\gamma}(g)$, $\mathcal{L}(g) = D^l_{\gamma^{-1}}(g) \otimes \mathbb{I}$ and $X(g)$, $Y(g)$, $D^r_{\gamma}(g)$ and $D^l_{\gamma^{-1}}(g)$ are irreducible projective representations (both $X(g)$ and $Y(g)$ have multiplier γ).

Proposition 3 (*Structure of an Elementary B Block*)**.** *Let B be an elementary B block (Definition 3.1). If $X(g) = D^r_{\gamma}(g)$ and $\overline{Y(g)} = D^l_{\gamma^{-1}}(g)$, then B is proportional to the tensor composed of the matrices*

$$B^{m,n} = |m\rangle\langle n| \ , \ m = 1, \ldots, dim(l), \ n = 1, \ldots, dim(r) \ .$$

Otherwise $B = 0$.

We have thus classified all tensors B that satisfy Eq. (13). There is however more information to be extracted from Theorem 2. According to Proposition 3, when projected to sectors corresponding to inequivalent representations, the tensor B is zero. This result, combined with the assumption that B is in CF imposes relations between the irreducible representations that comprise $\mathcal{R}(g)$, $\mathcal{L}(g)$ and $X(g)$:

Proposition 4. *Let B, $\mathcal{R}(g)$, $\mathcal{L}(g)$ and $X(g)$ be as in Theorem 2. Let $X_j(g) = \oplus_a X^a_j(g)$ be a block of $X(g)$ appearing in Eq. (14), consisting of irreducible projective representations $X^a_j(g)$. Let $\mathcal{R}(g) = \oplus_k (\mathbb{I} \otimes D^{r_k}_{\gamma}(g))$ and $\mathcal{L}(g) = \oplus_k (D^{l_k}_{\gamma^{-1}}(g) \otimes \mathbb{I})$, where $D^{r_k}_{\gamma}$ and $D^{l_k}_{\gamma^{-1}}$ are irreducible projective representations. Then the following hold:*

1. *For all k either there exist a and b such that $X^b_j(g) = D^{r_k}_{\gamma}(g)$ and $\overline{X^a_j(g)} = D^{l_k}_{\gamma^{-1}}(g)$, or the projection of the corresponding tensor B_j (a BNT element of B) to the sector k of the physical space is zero.*
2. *$\forall a \ \exists k$ such that $\overline{X^a_j(g)} = D^{l_k}_{\gamma^{-1}}(g)$.*
3. *$\forall a \ \exists k$ such that $X^a_j(g) = D^{r_k}_{\gamma}(g)$.*

The elementary block of B described in Proposition 3 is the same as the one used in [34]. Note that even in lattices of higher dimensionality each gauge field degree of freedom still connects two lattice sites. There:

$$B^{j;m,n} = \beta_j |j, m\rangle\langle j, n| \,, \tag{18}$$

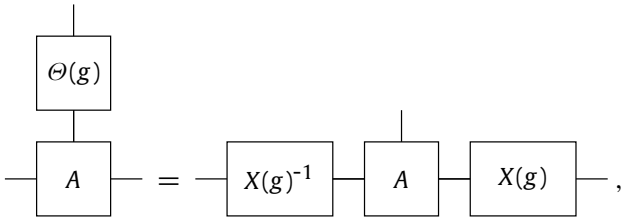
where β_j are arbitrary constants. The overall structure of the B tensor derived above admits more general structures than Eq. (18); these structures are recovered if for example, all blocks $X_j(g)$ appearing in $X(g)$ (Eq. (14)) are irreducible representations. In this case (since in Proposition 4 the index a can assume only one value), for all k $D^{l_k}_{\gamma^{-1}}(g) = \overline{D^{r_k}_{\gamma}(g)}$ and $\mathcal{H}_B$ takes the K–S form, as in Eq. (16).

In the following two propositions we consider adding a matter degree of freedom to a gauge field MPV with a local symmetry. We show that it is always possible to find a tensor A and a unitary representation $\Theta(g)$ (non-trivial ones) that couple to it:

Proposition 5. *Let B be in CFII and let $|\psi^N_B\rangle$ have a local symmetry with respect to $\mathcal{R}(g) \otimes \mathcal{L}(g)$ (as in Theorem 2). It is always possible to find a tensor A and a representation $\Theta(g)$ such that the corresponding matter and gauge field MPV $|\psi^N_{AB}\rangle$ has a local symmetry with respect to $\mathcal{R}(g) \otimes \Theta(g) \otimes \mathcal{L}(g)$ (Definition 4). In addition, the corresponding matter MPV - $|\psi^N_A\rangle$ - has a global symmetry with respect to $\Theta(g)$.*

For a restricted class of B tensors, *any* A and $\Theta(g)$ that couple to it (satisfy Definition 4) will have a global symmetry:

Proposition 6. *Let B, $\mathcal{R}(g)$ and $\mathcal{L}(g)$ be as in Theorem 2 and in addition let span$\{B^{k;m,n} \mid k, m, n\}$ contain the identity matrix (e.g.* Eq. (18)*). Let A and $\Theta(g)$ be such that the MPV generated by AB has a local symmetry with respect to $\mathcal{R}(g) \otimes \Theta(g) \otimes \mathcal{L}(g)$ (Definition 4). Then $|\psi^N_A\rangle$ has a global symmetry with respect to $\Theta(g)$. If in addition A is in CF with the same block structure as B (*Eq. (12)*), then A transforms as:*

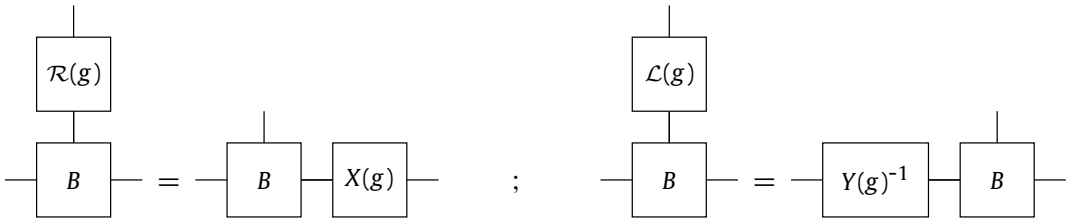


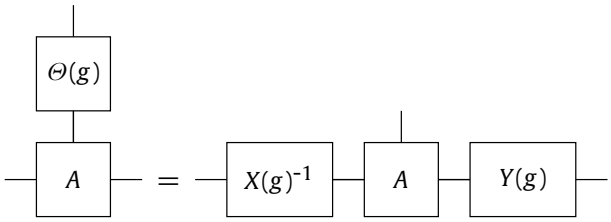
with the same $X(g)$ from Theorem 2.

The MPVs described above may be combined in a way that allows coupling matter and gauge fields such that each of them could be invariant on its own, as in the conventional well known scenarios of gauge theories. However, as we shall demonstrate in the next section, this is not the most general setting of a local symmetry involving these two building blocks.

3.3. Matter and gauge field MPV

We show that a local symmetry for a combined matter and gauge field MPV $|\psi^N_{AB}\rangle$ (defined in Section 2.3.3) generated by tensors A and B (in an appropriate form), implies the following transformation relations for A and B:





(19)

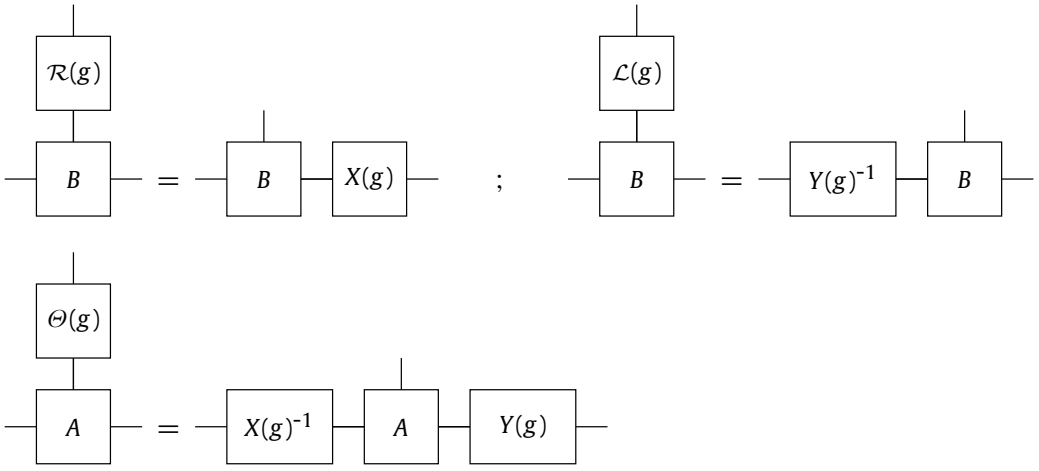
where $X(g)$ and $Y(g)$ are projective representations from the same cohomology class. As described in the previous section, the relation for B allows to infer the structure of the Hilbert space $\mathcal{H}_B$ associated with the gauge field degree of freedom. As before, $\mathcal{H}_B$ splits into right and left parts. The structure of the tensor B can be derived in the same way as in the previous section. Each elementary block of the tensor A, obtained by projecting Eq. (19) to irreducible representation spaces, satisfies a vector operator relation, and is therefore determined by the Wigner–Eckart theorem (Theorem 2.1).

In the general case, the structure described in this section allows for "unconventional" gauge symmetries where a local symmetry exists for the matter and gauge field MPV but none of the constituents has a symmetry on its own, i.e., the gauge field MPV does not have a local symmetry and the matter MPV does not have a global one. We construct an explicit example of such a case (see Proposition 11).

Finally we use the known results about global symmetries in MPV [44] to find a class of matter MPVs with a global symmetry that can be gauged by adding a gauge field degree of freedom. We shall now state the above results in detail.

Let $|\psi^N_{AB}\rangle$ be a MPV generated by tensors A and B and let $\mathcal{R}(g)$, $\Theta(g)$ and $\mathcal{L}(g)$ be as defined in Section 2.3.3.

Theorem 3 (*Matter and Gauge Field MPV with a Local Symmetry*)**.** *Let both BA and AB be normal tensors in CFII and let $\Theta(g)$ and $\mathcal{R}(g)$, $\mathcal{L}(g)$ be unitary and projective representations (with inverse multipliers) of a group G respectively. Let $|\psi^N_{AB}\rangle$ be a MPV with a local symmetry with respect to $\mathcal{R}(g)\otimes\Theta(g)\otimes\mathcal{L}(g)$ (Definition 4). Then there exist projective representations $X(g)$ and $Y(g)$ on $\mathbb{C}^{D_1}$ and $\mathbb{C}^{D_2}$ respectively, such that $X(g)$ has the same multiplier as $\mathcal{R}(g)$, and $Y(g)$ - the inverse multiplier to that of $\mathcal{L}(g)$. The tensors A and B transform as follows:*



(20)

(21)

In the following proposition we show that given arbitrary tensors A and B, generating a MPV $|\psi^N_{AB}\rangle$, it is possible to describe the same MPV as a linear combination of MPVs that satisfy the normality condition in Theorem 3:

Proposition 7. *Let $|\psi^N_{AB}\rangle$ be a MPV generated by arbitrary tensors A and B. Then there exist tensors $\{A_\chi\}$ and $\{B_\chi\}$, and there exists $b\in\mathbb{N}$ such that for all χ both $A_\chi B_\chi$ and $B_\chi A_\chi$ are normal tensors and $\forall N\in\mathbb{N}$ $|\psi^N_{AB_{\times b}}\rangle=\sum_\chi \mu^N_\chi|\psi^N_{A_\chi B_\chi}\rangle$, where μ_χ are constants and $AB_{\times b}$ is the tensor obtained by blocking b copies of the tensor AB.*

Next we show that if $|\psi^N_{AB}\rangle = \sum_\chi \mu^N_\chi |\psi^N_{A_\chi B_\chi}\rangle$ has a local symmetry with respect to $\mathcal{R}(g)\otimes\Theta(g)\otimes\mathcal{L}(g)$, then every normal component $|\psi^N_{A_\chi B_\chi}\rangle$ must have the same symmetry. We can then apply Theorem 3 to each of the components.

Proposition 8. *Let $|\psi^N_{AB}\rangle = \sum_\chi \mu^N_\chi |\psi^N_{A_\chi B_\chi}\rangle$ where both $A_\chi B_\chi$ and $B_\chi A_\chi$ are normal tensors. Let O be a local operator acting on a fixed number of adjacent sites. If $\forall N$ O leaves the MPV invariant:*

$$O\otimes\mathbb{I}|_{rest}|\psi^N_{AB}\rangle = |\psi^N_{AB}\rangle\ ,$$

then O leaves every component invariant:

$$O\otimes\mathbb{I}|_{rest}|\psi^N_{A_\chi B_\chi}\rangle = |\psi^N_{A_\chi B_\chi}\rangle\ \forall\chi\ .$$

Having derived Eq. (20), Proposition 2 can be applied to determine the structure of the Hilbert space $\mathcal{H}_B$. As in the case of a gauge field MPV discussed in the previous section, we are free to assume $X(g)$ and $Y(g)$ are block diagonal in irreducible representations:

Remark 3.5. In Theorem 3 we are free to choose similarity transformations for $X(g)$ and $Y(g)$ independently. Given A, B, $\mathcal{R}(g)$, $\Theta(g)$, $\mathcal{L}(g)$, $X(g)$ and $Y(g)$ that satisfy Eq. (20) and Eq. (21) we can redefine A and B:

$$A^{j,m}\mapsto\tilde{A}^{j,m}=U^{-1}A^{j,m}V\ ,\quad B^{k;m,n}\mapsto\tilde{B}^{k;m,n}=V^{-1}B^{k;m,n}U\ ,$$

with any invertible matrices U and V of fitting dimensions. The new tensors generate the same MPV $|\psi^N_{AB}\rangle$ and transform as in Theorem 3 with $X(g)$ and $Y(g)$ replaced by $\tilde{X}(g)=U^{-1}X(g)U$ and $\tilde{Y}(g)=V^{-1}Y(g)V$.

Definition 3.2 (*Elementary A Block*)**.** An elementary block of the tensor A is one which satisfies Eq. (21), where $\Theta(g)$, $X(g)$ and $Y(g)$ are all irreducible projective representations.

By bringing all of the representations appearing in Eqs. (20) and (21) to block diagonal form (using Remark 2.2 on the physical representations and Remark 3.5 on the virtual ones), and projecting Eqs. (20) and (21) to irreducible sectors of the physical and virtual Hilbert spaces (as explained in Section 3.2), we may reduce Eq. (20) and Eq. (21) to the cases of elementary blocks of B and of A respectively.

We have seen in Section 3.2 that Eq. (20) determines the tensor B given $\mathcal{R}(g)$, $\mathcal{L}(g)$, $X(g)$ and $Y(g)$ (Proposition 4). We now show that Eq. (21) determines the tensor A given $\Theta(g)$, $X(g)$ and $Y(g)$.

Proposition 9. *Let A be an elementary block (Definition 3.2), with $\Theta(g)=D^{j_0}(g)$, $X(g)=D^j_\gamma(g)$ and $Y(g)=D^l_{\gamma^{-1}}(g)$. Then A is built out of Clebsch–Gordan coefficients and has the form:*

$$A^M=\sum_{J\in\mathfrak{J}:D^J=D^{j_0}}\alpha_J\sum_{m,n}\left\langle J,M\,|\,\bar{j},m;l,n\right\rangle|m\rangle\langle n|\ ,$$

where $\mathfrak{J}$ is the set of irreducible representation indices appearing in the decomposition of $\overline{D^j_\gamma(g)}\otimes D^l_{\gamma^{-1}}(g)$ into irreducible representations, $\left\langle\bar{j},m:l,n\,|\,J,M\right\rangle$ are the Clebsch–Gordan coefficients of the decomposition, $\overline{D^j_\gamma(g)}$ is the complex conjugate representation to $D^j_\gamma(g)$ and α_J are arbitrary constants.

Proposition 9 was shown in [44] in the context of MPS with a global symmetry.

The relation between the irreducible projective representations appearing in $\mathcal{R}(g)$ ($\mathcal{L}(g)$) and $X(g)$ ($Y(g)$) is characterized by the following:

Proposition 10. *Let AB and BA be normal tensors and let B satisfy* Eq. (20) *with $\mathcal{R}(g)=\oplus_k(\mathbb{I}\otimes D^{r_k}_\gamma(g))$, $\mathcal{L}(g)=\oplus_k(D^{l_k}_{\gamma^{-1}}(g)\otimes\mathbb{I})$, $Y(g)=\oplus_a Y^a(g)$ and $X(g)=\oplus_b X^b(g)$, where $D^{r_k}_\gamma$, $D^{l_k}_{\gamma^{-1}}$, Y^a and X^b are irreducible projective representations, then*

1. *For all k either there exist a and b such that* $X^b(g) = D^{r_k}_\gamma(g)$ *and* $\overline{Y^a(g)} = D^{l_k}_{\gamma^{-1}}(g)$ *or the projection of the tensor B to the sector k of the physical space is zero (and it can be discarded).*
2. $\forall a\ \exists k$ *such that* $\overline{Y^a(g)} = D^{l_k}_{\gamma^{-1}}(g)$.
3. $\forall b\ \exists k$ *such that* $X^b(g) = D^{r_k}_\gamma(g)$.

By constructing tensors A and B that transform as in Theorem 3 with $X(g) \neq Y(g)$ we show the existence of matter and gauge field MPVs which have a local symmetry but for which the corresponding matter MPV does not have a global symmetry, nor does the gauge field MPV have a local one:

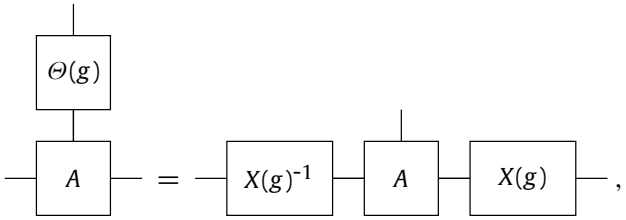
Proposition 11. *There exist tensors A and B such that* $|\psi_{AB}\rangle$ *has a local symmetry with respect to* $\mathcal{R}(g) \otimes \Theta(g) \otimes \mathcal{L}(g)$*, but* $|\psi_A\rangle$ *does not have a global symmetry with respect to* $\Theta(g)$*. In addition* $\mathcal{R}(g) \otimes \mathcal{L}(g)|\psi_B\rangle \neq |\psi_B\rangle$.

We review known results about MPV with global symmetry [44]. Let A be a tensor in CFII:

$$A^i = \oplus_{j=1}^{n} \oplus_{q=1}^{r_j} \mu_{j,q} A^i_j \,, \tag{22}$$

where $\{A_j\}$ are normal tensors in CFII forming a BNT of A (Definition 2.7) and $\mu_{j,q}$ are constants.

Theorem 4. *A tensor A in CFII which generates a MPV with a global symmetry with respect to a representation* $\Theta(g)$ *of a connected Lie group G, transforms under the representation matrix as:*



(23)

where $X(g)$ *has the same block structure as A:*

$$X(g) = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} X_j(g) \,, \tag{24}$$

and where each block $X_j(g)$ *is a projective representation, in the general case, for different j values* $X_j(g)$ *belong to different cohomology classes.*

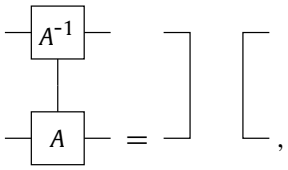
In the case when all $X_j(g)$ obtained in Theorem 4 are from the same cohomology class, we can find a gauge field tensor B and projective representations $\mathcal{R}(g)$ and $\mathcal{L}(g)$ that gauge the symmetry:

Proposition 12. *Let A be a tensor in CFII generating a MPV with a global symmetry i.e., satisfying Theorem 4. Let* $X(g)$ *(in* Eq. (23)*) be a projective representation (i.e. all* $X_j(g)$ *in* Eq. (24) *are in the same cohomology class). Then there exist a tensor B and projective representations* $\mathcal{R}(g)$ *and* $\mathcal{L}(g)$ *with inverse multipliers such that both local symmetries: Definition 4 for* $|\psi^N_{AB}\rangle$ *and Definition 3 for* $|\psi^N_B\rangle$ *are satisfied.*

4. MPV with a global symmetry

In the next section we shall present the derivation of the previously described results. Before that, however, we review MPVs basics not covered in the formalism section, needed for the derivation of the classification of MPVs with a global symmetry, originally shown in [44]. In order for the paper to be self contained, we derive the result from the fundamental theorem of MPV (see Theorem 4.1), following [38] and references therein.

Proposition 4.1. *Definition 2.2 is equivalent to the existence of a one-sided inverse tensor A^{-1} which satisfies:*



that is:

$$\sum_i A^i_{\alpha\beta}(A^{-1})^i_{\alpha\beta} = \delta_{\alpha,\alpha'}\delta_{\beta,\beta'}$$

Definition 4.1 (*Span of Matrix Products*)**.** For a tensor A with bond dimension D let $S_L \subseteq \mathcal{M}_{D\times D}$ be the space spanned by all possible L-fold matrix products:

$$\mathcal{S}_L := span\left\{A^{i_1}A^{i_2}\dots A^{i_L} \mid i_1, i_2, \dots, i_L = 1, \dots, d\right\} .$$

Definition 4.2. Let $\Gamma^L_A : \mathcal{M}_{D\times D} \to \mathcal{H}^{\otimes L}$ be defined by:

$$\Gamma^L_A(X) = \sum \mathrm{Tr}\left(XA^{i_1}A^{i_2}\dots A^{i_L}\right)|i_1 i_2 \dots i_L\rangle .$$

For a normal tensor, according to Definition 2.4, for L large enough, $S_L = \mathcal{M}_{D\times D}$. For tensors in CF the following holds:

Proposition 4.2 (*Span Property of BNT*)**.** *Let A be in CF with each block being a unique element of its BNT, i.e. there is no q summation in* Eq. (3)*. Then for L large enough, $\mathcal{S}_L$ is the entire matrix algebra $\mathcal{M} := \oplus_{j=1}^m \mathcal{M}_{D_j\times D_j}$ where $\mathcal{M}_{D_j\times D_j}$ is the algebra of $D_j \times D_j$ matrices and D_j is the bond dimension of A_j* [37].

Proposition 4.3. *Let A be a tensor consisting of block diagonal matrices: $A^i \in \mathcal{M} := \oplus_j^m \mathcal{M}_{D_j\times D_j}$, and let $\mathcal{S}_L$ and Γ^L_A be as in Definitions 4.1 and 4.2 respectively. Then $\mathcal{S}_L = \mathcal{M}$ iff $\Gamma^L_A|_{\mathcal{M}}$ is injective.*

Proof. Assume injectivity of $\Gamma^L_A|_{\mathcal{M}}$, then any element $X \in \mathcal{S}^\perp \cap \mathcal{M}$ satisfies $\Gamma^L_A(X^\dagger) = 0$ because the coefficients of the vector $\Gamma^L_A(X^\dagger)$ are inner products of X with elements in $\mathcal{S}$. This implies $X = 0$. If $\mathcal{S} = \mathcal{M}$, then for every non zero $X \in \mathcal{M}$, $X^\dagger$ has a non vanishing inner product with at least one element $A^{i_1}A^{i_2}\dots A^{i_L}$, and therefore $\Gamma^L_A(X)$ is non zero. □

Proposition 4.4. *For a tensor A in CF as in* Eq. (3)*, for L large enough the space $\mathcal{S}_L$ (Definition 4.1) has the form:*

$$\mathcal{S}_L = \left\{\oplus_{j=1}^m \oplus_{q=1}^{r_j} \mu^L_{j,q} V^{-1}_{j,q} M_j V_{j,q} \mid M_j \in \mathcal{M}_{D_j\times D_j}\right\} . \tag{25}$$

Proof. Consider a tensor $\tilde{A}$ which consists of the BNT of A without multiplicities (as in Proposition 4.2). An element $S = \oplus_{j=1}^m \oplus_{q=1}^{r_j} \mu^L_{j,q} V^{-1}_{j,q} M_j V_{j,q}$ in $\mathcal{S}_L$ is obtained by taking the same linear combination of the matrix products $A^{i_1}A^{i_2}\dots A^{i_L}$ as the one which generates $\tilde{S} = \oplus_{j=1}^m M_j$ from the matrix products $\tilde{A}^{i_1}\tilde{A}^{i_2}\dots\tilde{A}^{i_L}$. □

Proposition 4.5. *Let $\{A_j\}_{j=1}^m$ be a BNT of A, and let each A_j appear in A with no multiplicities, i.e. $A^i = \oplus_{j=1}^m \nu_j A^i_j$. For L large enough the image of the algebra of block diagonal matrices $\mathcal{M} := \oplus_{j=1}^m \mathcal{M}_{D_j\times D_j}$, where D_j is the bond dimension of A_j, under the map Γ^L_A is a direct sum:*

$$\Gamma^L_A(\mathcal{M}) := \left\{\Gamma^L_A(X) \mid X \in \mathcal{M}\right\} = \oplus_{j=1}^m \Gamma^L_{A_j}(\mathcal{M}_{D_j\times D_j}) .$$

In particular $\sum_{j=1}^m \Gamma^L_{A_j}(X_j) = 0$ implies $X_j = 0 \ \ \forall j = 1, \dots, m$. [37]

Proposition 4.5 allows us to prove the following lemma:

Lemma 4.1. *Let A be a tensor in CF with BNT $\{A_j\}$, and let S and T be tensors with the exact same block structure as A:*

$$A^i = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} \mu_{jq} V_{j,q}^{-1} A_j^i V_{j,q}$$

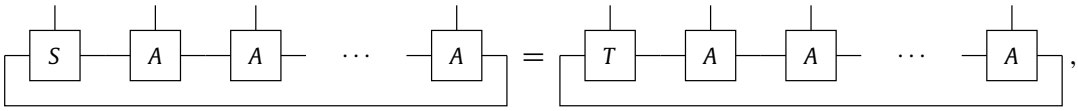
$$S^i = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} \mu_{jq} V_{j,q}^{-1} S_j^i V_{j,q}$$

$$T^i = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} \mu_{jq} V_{j,q}^{-1} T_j^i V_{j,q} \, .$$

If the following equality holds for any length N:

$$\sum_{\{i\}} \mathrm{Tr}\left(S^{i_1} A^{i_2} \ldots A^{i_N}\right) |i_1, i_2, \ldots, i_N\rangle = \sum_{\{i\}} \mathrm{Tr}\left(T^{i_1} A^{i_2} \ldots A^{i_N}\right) |i_1, i_2, \ldots, i_N\rangle \, , \tag{26}$$

which in tensor notation reads:



then $S = T$.

Proof. Plugging in the block structure of the tensors into Eq. (26) we obtain:

$$\begin{aligned} 0 &= \sum_{\{i\}} \mathrm{Tr}\left(\oplus_{j=1}^{m} \oplus_{q=1}^{r_j} \mu_{j,q}^N \left[T_j^{i_1} - S_j^{i_1}\right] A_j^{i_2} \ldots A_j^{i_N}\right) |i_1, i_2, \ldots, i_N\rangle \\ &= \sum_{j=1}^{m} \sum_{q=1}^{r_j} \mu_{j,q}^N \sum_{\{i\}} \mathrm{Tr}\left(\left[T_j^{i_1} - S_j^{i_1}\right] A_j^{i_2} \ldots A_j^{i_N}\right) |i_1, i_2, \ldots, i_N\rangle \, . \end{aligned}$$

Plugging in the definition of the map Γ_A (Definition 4.2)

$$\sum_{j=1}^{m} \sum_{i_1} \Gamma_{A_j}^{N-1} \left(\sum_{q=1}^{r_j} \mu_{j,q}^N \left[T_j^{i_1} - S_j^{i_1}\right] \right) \otimes |i_1\rangle = 0 \, .$$

According to Proposition 4.5, for N large enough ($\geq L_0$) we have for all i_1 and all j

$$\sum_{q=1}^{r_j} \mu_{j,q}^N \left[T_j^{i_1} - S_j^{i_1}\right] = 0 \, .$$

For all j, since $\{\mu_{j,q}\}_{q=1}^{r_j}$ are non-zero, there exists an $N \geq L_0$ such that $\sum_{q=1}^{r_j} \mu_{j,q}^N \neq 0$. Therefore for all j we have:

$$T_j^i = S_j^i \, . \qquad \square \tag{27}$$

We review the fundamental theorem of MPV [38] and apply it to the case of a MPV with a global symmetry.

Proposition 4.6. [38] *Let A and B be tensors in CF (*Eq. (3)*) with BNT $\{A_j\}_{j=1}^{g_a}$ and $\{B_k\}_{k=1}^{g_b}$ respectively. If for all N the tensors A and B generate MPVs proportional to each other, then $g_a = g_b$ and for every j there is a unique $k(j)$, a unitary matrix X_j and a phase $e^{i\phi_j}$ such that:*

$$A_j^i = e^{i\phi_j} X_j^{-1} B_{k(j)}^i X_j \, .$$

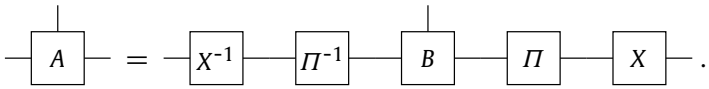
Remark 4.1. Note that X_j are determined up to a phase.

Proposition 4.6 was proved in [38] and was used to prove the following:

Theorem 4.1 (*The Fundamental Theorem of MPV*)**.** *Let two tensors A and B in CF (CFII) generate the same MPV for all N. Then they have the same block structure, and there exists an invertible (unitary) matrix X:*

$$X = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} X_j \,, \tag{28}$$

which is block diagonal, with the same block structure as A, and a permutation matrix Π between the blocks, such that:

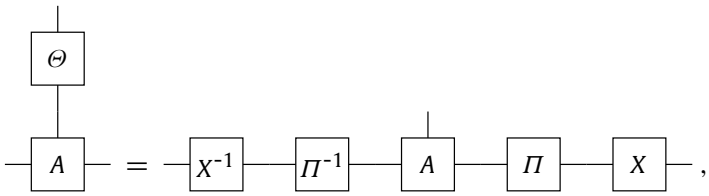


We now apply the fundamental theorem of MPV to the case when a MPV generated by a tensor A in CFII is invariant under the action of the same unitary operator on every site:

Corollary 4.1. *Let A be a tensor in CFII (*Eq. (3)*) generating a MPV with a global invariance under a unitary Θ:*

$$\Theta^{\otimes N} |\psi_A^N\rangle = |\psi_A^N\rangle \,,$$

then A transforms under the unitary matrix as:



*where X is a unitary matrix with the same block structure as A, and is unitary in each block (*Eq. (28)*), and Π is a permutation between the j blocks of A (it does not permute the q blocks).*

Proof. The tensor $\tilde{A}$ consisting of the matrices $\tilde{A}^i := \sum_{i'} \Theta_{i,i'} A^{i'}$ generates $\Theta^{\otimes N} |\psi_A^N\rangle$. Before finishing the proof, we shall now prove the following lemma:

Lemma 4.2. *Let $\{A_j\}$ be the BNT of A, then the tensors $\{\tilde{A}_j\}$ composed of the matrices $\tilde{A}_j^i = \sum_{i'} \Theta_{i,i'} A_j^{i'}$ form a BNT of $\tilde{A}$, and $\tilde{A}$ is in CFII.*

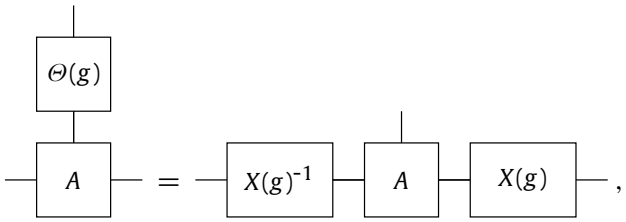
Proof. $\tilde{A}_j$ are normal tensors and in CFII because a unitary mixture of the Kraus operators gives the same CP map (Proposition 2.3), and they are a basis because $\{A_j\}$ is. □

We can now apply the fundamental theorem of MPV to A and $\tilde{A}$. In this case, however, because the coefficients $\mu_{j,q}$ in Eq. (3) are the same for A and $\tilde{A}$, Π permutes only between j blocks. □

Next we apply the above to a MPV with a global symmetry as in Definition 2:

$$\Theta(g)^{\otimes N} |\psi_A^N\rangle = |\psi_A^N\rangle \,.$$

Theorem 4. *A tensor A in CFII which generates a MPV with a global symmetry with respect to a representation $\Theta(g)$ of a connected Lie group G, transforms under the representation matrix as:*



(23)

where $X(g)$ has the same block structure as A:

$$X(g) = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} X_j(g)\,, \tag{24}$$

and where each block $X_j(g)$ is a projective representation, in the general case, for different j values $X_j(g)$ belong to different cohomology classes.

Proof. According to Corollary 4.1, for every $g \in G$ we have:

$$\sum_{i'} \Theta(g)_{i,i'} A^{i'} = X(g)^{-1} \Pi(g)^{-1} A^{i} \Pi(g) X(g)\,. \tag{29}$$

Consider the action of the group element $gh \in G$ in two ways using Eq. (29):

$$\begin{aligned} X(gh)^{-1}\Pi(gh)^{-1}A^{i}\Pi(gh)X(gh) &= \sum_{i'} \Theta(gh)_{i,i'}A^{i'} \\ &= \sum_{i',k} \Theta(g)_{i,k}\Theta(h)_{k,i'}A^{i'} \\ &= \sum_{k} \Theta(g)_{i,k}X(h)^{-1}\Pi(h)^{-1}A^{k}\Pi(h)X(h) \\ &= X(h)^{-1}\Pi(h)^{-1}X(g)^{-1}\Pi(g)^{-1}A^{i}\Pi(g)X(g)\Pi(h)X(h)\,. \end{aligned}$$

Taking the L-fold product of the LHS and RHS for different indices $i_1, i_2, \ldots, i_L$ we obtain:

$$\begin{aligned} &X(gh)^{-1}\Pi(gh)^{-1}\left(A^{i_1}A^{i_2}\ldots A^{i_L}\right)\Pi(gh)X(gh) \\ &\quad = X(h)^{-1}\Pi(h)^{-1}X(g)^{-1}\Pi(g)^{-1}\left(A^{i_1}A^{i_2}\ldots A^{i_L}\right)\Pi(g)X(g)\Pi(h)X(h)\,. \end{aligned} \tag{30}$$

We shall now prove the following lemma, and then continue with the proof.

Lemma 4.3. *$\Pi(g)$ is a representation of G and is therefore the trivial one.*

Proof. According to Proposition 4.4, by taking appropriate linear combinations of Eq. (30) we can obtain:

$$\begin{aligned} &X(gh)^{-1}\Pi(gh)^{-1}\left(\Delta[j]\right)\Pi(gh)X(gh) \\ &\quad = X(h)^{-1}\Pi(h)^{-1}X(g)^{-1}\Pi(g)^{-1}\left(\Delta[j]\right)\Pi(g)X(g)\Pi(h)X(h)\,, \end{aligned} \tag{31}$$

where $\Delta[j_0]$ is a matrix consisting of multiples of $\mathbb{I}$ in the j_0 block and zero in all the rest: $\Delta[j_0] := \oplus_{j=1}^{m}\oplus_{q=1}^{r_j}\mu_{j,q}^{L}\delta_{j,j_0}\mathbb{I}_{D_j\times D_j}$. This is achieved by setting $M_j = \delta_{j,j_0}\mathbb{I}$ in Eq. (25). Denote by $g(j)$ the image of the block j under the permutation $\Pi(g)$, then $\Pi(g)^{-1}\Delta[j]\Pi(g) = \Delta[g^{-1}(j)]$. Plugging this into Eq. (31) we get:

$$\begin{aligned} LHS &= X(gh)^{-1}\left(\Delta[(gh)^{-1}(j)]\right)X(gh) \\ &= \Delta[(gh)^{-1}(j)] = \\ RHS &= X(h)^{-1}\Pi(h)^{-1}X(g)^{-1}\left(\Delta[g^{-1}(j)]\right)X(g)\Pi(h)X(h) \\ &= X(h)^{-1}\Pi(h)^{-1}\left(\Delta[g^{-1}(j)]\right)\Pi(h)X(h) \\ &= \Delta[h^{-1}(g^{-1}(j))]\,, \end{aligned}$$

where in each step the Xs commute with the Δs because they have the same block structure and the Δs are proportional to $\mathbb{I}$ in each block. We conclude that $(gh)^{-1}(j)$ and $h^{-1}(g^{-1}(j))$ are the same block number and therefore $\Pi(g)$ is a group homomorphism. It remains to show that $\Pi(g)$ depends on g

smoothly. From Eq. (29) we obtain:

$$X(g)^{-1}\Pi(g)^{-1}A^{i_1}A^{i_2}\dots A^{i_L}\Pi(g)X(g) = \sum_{\{i'\}}\left(\Theta(g)_{i_1,i'_1}A^{i'_1}\right)\left(\Theta(g)_{i_2,i'_2}A^{i'_2}\right)\dots\left(\Theta(g)_{i_L,i'_L}A^{i'_L}\right). \tag{32}$$

As above, we can take a linear combination of the As to get a $\Delta[j]$ between the permutations in the LHS. Knowing how the permutation acts on each $\Delta[j]$ determines $\Pi(g)$ completely. The Xs on the LHS commute with all $\Delta[j]$ as before. The RHS will then be a linear combination of $\{\Theta(g)A\}$, and will thus depend on g smoothly. Since we assumed G is a connected Lie group we conclude that $\Pi(g) \equiv \mathbb{I}$. □

We now repeat the step leading to Eq. (31) but this time with an arbitrary matrix M in the j block: $\Delta^M_{j_0} := \oplus_{j=1}^{m}\oplus_{q=1}^{r_j}\delta_{j,j_0}\mu^L_{j,q}M$. Eq. (31) becomes:

$$X(gh)^{-1}\left(\Delta^M_j\right)X(gh) = X(h)^{-1}X(g)^{-1}\left(\Delta^M_j\right)X(g)X(h)\,.$$

This means that for any j block we have:

$$\oplus_{q=1}^{r_j}\mu^L_{j,q}X_j(gh)^{-1}MX_j(gh) = \oplus_{q=1}^{r_j}\mu^L_{j,q}X_j(h)^{-1}X_j(g)^{-1}MX_j(g)X_j(h)\,.$$

We see that $X_j(g)X_j(h)(X_j)^{-1}(gh)$ commutes with every matrix M and is therefore proportional to the identity. $X_j(g)$ is therefore a projective representation. □

Remark 4.2. Note that different blocks of $X(g)$ can belong to different equivalence classes of projective representations. We could construct such an example by taking the direct sum of two normal tensors A and $\tilde{A}$, which transform under a given representation $\Theta(g)$ with $X(g)$ and $\tilde{X}(g)$, projective representations from different cohomology classes. $X(g)\oplus\tilde{X}(g)$ is then not a projective representation because $X(gh)\oplus\tilde{X}(gh)$ differs from $X(g)X(h)\oplus\tilde{X}(g)\tilde{X}(h)$ by a diagonal matrix and not a scalar one.

5. Derivation and proofs of the results

In this section we prove the theorems stated in Section 3.

5.1. Matter MPV with local symmetry

Proposition 1. *Let $\mathcal{H}$ be a finite dimensional Hilbert space and let $\Theta : g \mapsto \Theta(g)$ be a representation on $\mathcal{H}$. Let $|\psi^N\rangle \in$ be a vector with a local symmetry, i.e.*

$$\Theta(g_1)\otimes\Theta(g_2)\otimes\dots\Theta(g_N)|\psi^N\rangle = |\psi^N\rangle, \quad \forall g_1, g_2, \dots, g_N \in G\,.$$

Then $|\psi^N\rangle \in {\mathcal{H}_0}^{\otimes N}$, where $\mathcal{H}_0 \subset \mathcal{H}$ is the subspace on which $\Theta(g)$ acts trivially.

Proof. Write $|\psi^N\rangle$ in the irreducible representation basis which satisfies:

$$\Theta(g)|j, m\rangle = \sum_n D^j(g)_{n,m}|j, n\rangle\,,$$

where $D^j(g)$ are irreducible representation matrices.

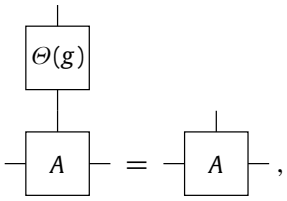
$$|\psi^N\rangle = \sum c_{j_1,m_1,\dots,j_N,m_N}|j_1, m_1, \dots, j_N, m_N\rangle\,.$$

The local symmetry condition implies:

$$\sum_{n_1} D^{j_1}(g)_{m_1,n_1}c_{j_1,n_1,\dots,j_N,m_N} = c_{j_1,m_1,\dots,j_N,m_N}\,,$$

which means that the vector of coefficients $\overrightarrow{c}_{j_1,(\cdot),\dots,j_N,m_N}$ is either zero or an invariant subspace of $D^{j_1}(g)$, in which case $D^{j_1}(g)$ is the trivial representation. This implies that the coefficients $c_{j_1,m_1,\dots,j_N,m_N}$ are zero whenever any one of the j_ks corresponds to a non trivial representation. □

Theorem 1. *Let A be a tensor in CF generating a MPV with a local symmetry with respect to a representation $\Theta(g)$ (Definition 1). Then for all $g \in G$ the tensor A satisfies:*



i.e., for all $i = 1, \ldots, d_A$: $\sum_{i'} \Theta(g)_{ii'} A^{i'} = A^i$.

Proof. We apply Lemma 4.1 with $S^i := \sum_{i'} \Theta(g)_{ii'} A^{i'}$ and $T^i := A^i$. □

Remark 5.1. We have never used any properties of $\Theta(g)$ as a representation. The same proof is valid for any operator Θ.

According to Remark 2.2, the MPV generated by A can be written in terms of a tensor $\tilde{A}$, composed of the matrices $\{\tilde{A}^{j,m}\}$, corresponding to the irreducible representation basis $\{|j, m\rangle\}$ on which $\Theta(g)$ acts as $\Theta(g)|j, m\rangle = \sum_n D^j(g)_{n,m}|j, n\rangle$. According to Corollary 2.1, $\tilde{A}$ is also in CF. Applying Theorem 1 to $\tilde{A}$ leads to the following:

Corollary 1. *The matrices $\tilde{A}^{j,m}$ are non-zero only for j such that $D^j(g) \equiv \mathbb{I}_{1\times 1}$.*

Proof. From Theorem 1 we deduce that each vector of matrix elements of A: $\vec{A}^j_{\alpha,\beta} = \left(A^{j,1}_{\alpha,\beta}, A^{j,2}_{\alpha,\beta}, \ldots, A^{j,dim(j)}_{\alpha,\beta}\right)^T$ is invariant under $D^j(g)$ for all $g \in G$. This implies that either $\vec{A}^j_{\alpha,\beta}$ is zero or that $D^j(g)$ is the one dimensional trivial representation. □

5.2. Pure gauge field MPV

In order to prove Theorem 2 we shall proceed as in Section 4: we shall first prove a lemma which describes the case when $\mathcal{R}$ and $\mathcal{L}$ are just unitary operators, and later use that to prove the case when they are representations.

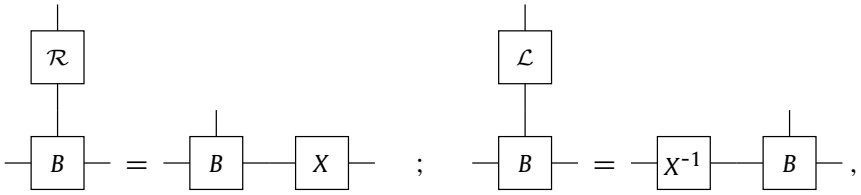
Lemma 5.1. *Let B be a tensor in CFII:*

$$B^i = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} \mu_{j,q} B^i_j \,,$$

and let $\mathcal{R}$ and $\mathcal{L}$ be two unitary operators such that for all K

$$\mathcal{R}^{[K]} \mathcal{L}^{[K+1]} |\psi_B^N\rangle = |\psi_B^N\rangle \,.$$

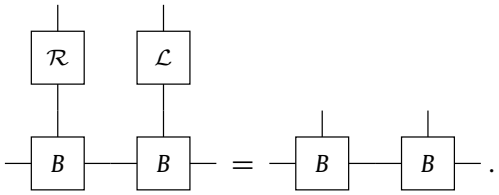
Then B transforms under the unitary matrices as follows:



(33)

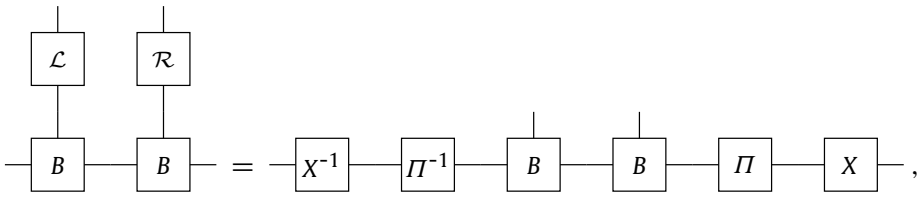
where X is a unitary matrix with the same block structure as B^i, as in Eq. (28).

Proof. Applying Theorem 1 (recall Remark 5.1) to the tensor BB and the unitary $\mathcal{R} \otimes \mathcal{L}$ (BB is in CF if B is in CF), we obtain:



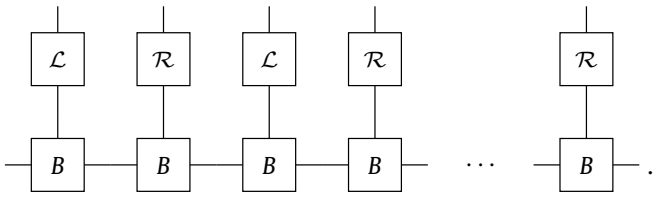
(34)

Applying the pair of operators to every site on the chain (for even N) we conclude that the MPV is invariant under the global application of the operators in reversed order: $(\mathcal{L} \otimes \mathcal{R})^{\otimes N} |\psi_B^{2N}\rangle = |\psi^2 N_B\rangle$. Using Corollary 4.1 we obtain:

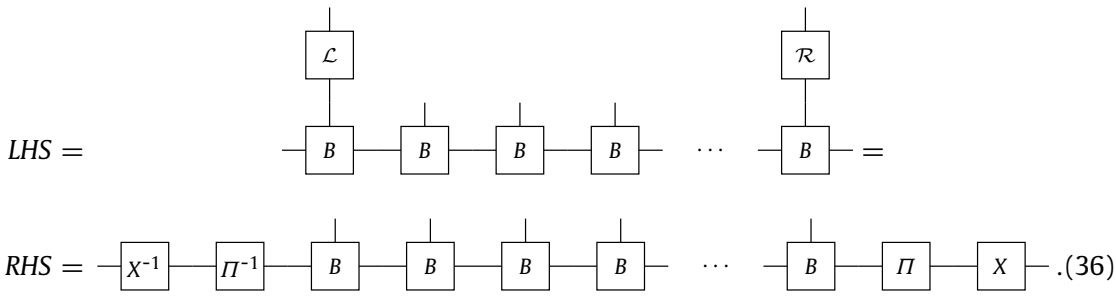


(35)

where X is unitary and Π is a permutation, as in Corollary 4.1. Next consider the following tensor:

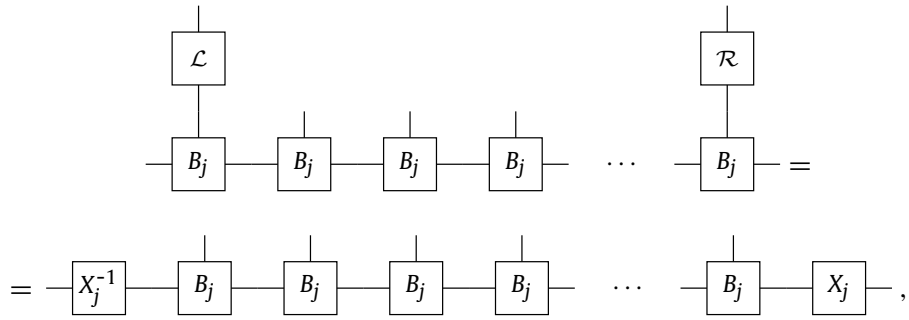


According to Eq. (34) this tensor is equal to the LHS of the following, and according to Eq. (35) — to the RHS:

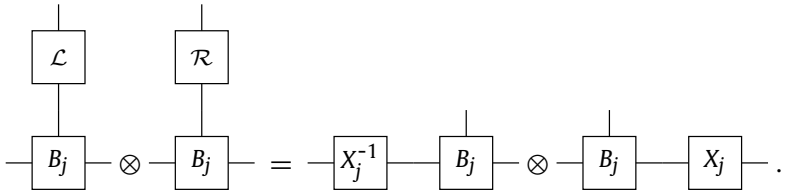


(36)

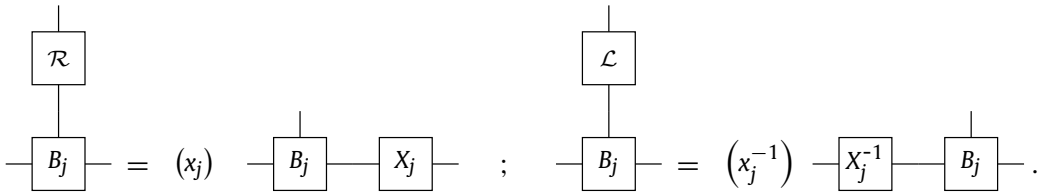
Using the same argument as in Eq. (31), we show that the permutation must act trivially: use Proposition 4.4 on the string of consecutive Bs, excluding the extreme right and left ones, to obtain multiples of $\mathbb{I}$ in a single j block and zeros elsewhere. Note that $\mathcal{R}$ and $\mathcal{L}$ do not change the block structure of the tensors they act on. Now compare the RHS with the LHS block-wise, if Π acts non trivially on a block j, then we get that $B_j B_j$ is zero, which is a contradiction to B_j being normal. Next, having eliminated the possibility of a permutation, project Eq. (36) to any (j, q) block to obtain:



where B_j is a normal tensor by assumption. We can now apply the inverse on the string of Bs in the middle (BB is normal if B is normal) to obtain:

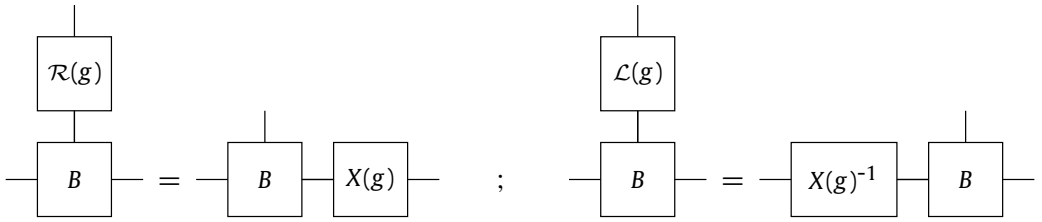


According to Remark 4.1, the matrices X_j are determined up to a constant. We now choose a representative from the projective unitary class of X_j. The above implies that for any such choice there is a constant x_j such that:



Therefore the desired X is $X = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} x_j X_j$. □

Theorem 2 (*Gauge field MPV with a local symmetry*)**.** *A tensor B in CFII which generates a MPV that has a local symmetry with respect to $\mathcal{R}(g) \otimes \mathcal{L}(g)$ where $\mathcal{R}(g)$ and $\mathcal{L}(g)$ are projective representations with inverse multipliers (Definition 3), transforms under the representation matrices as:*

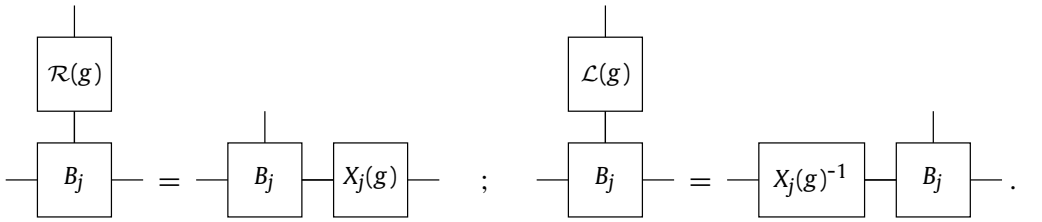


(13)

where $X(g)$ is a projective representation of G with the same multiplier as $\mathcal{R}(g)$ and with the same block structure as B (Eq. (12))*:*

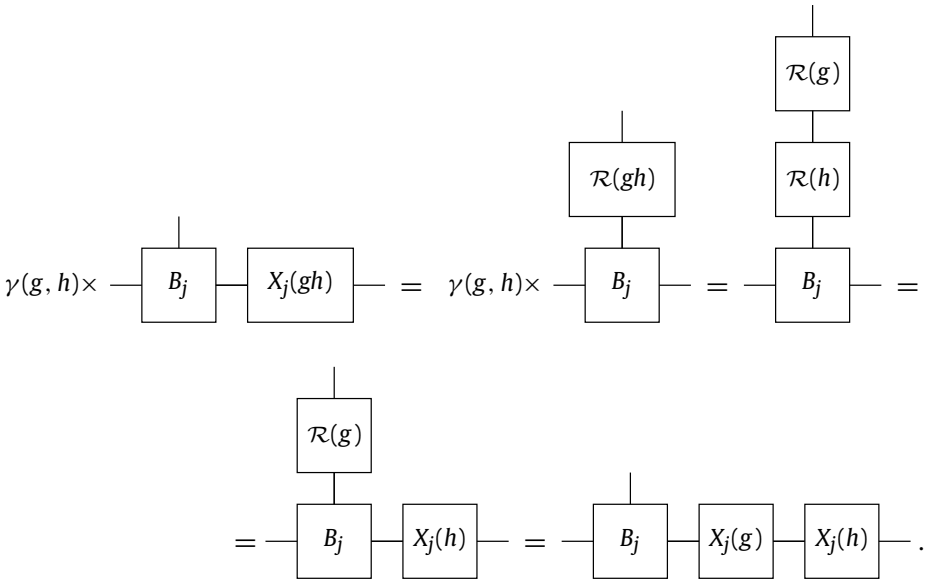
$$X(g) = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} X_j(g)\,. \tag{14}$$

Proof. As we have seen in the proof of Lemma 5.1, Eq. (33) holds for each block of B, so for every group element $g \in G$ we have:



(37)

We write the action of the group element $\mathcal{R}(gh)$ on B in two ways:



Now by contracting with the tensor $B_jB_j \dots B_j$ from the left, and taking the appropriate linear combination which results in the identity matrix (B_j is normal), we obtain $\gamma(g,h)X_j(gh) = X_j(g)X_j(h)$. This means that for all j $X_j(g)$ is a projective representation with the same multiplier as $\mathcal{R}(g)$ (γ). Therefore $X(g)$ is a projective representation. □

Proposition 2 (*Structure of $\mathcal{H}_B$*)**.** *Given a tensor B, projective representations $\mathcal{R}(g)$, $\mathcal{L}(g)$ with inverse multipliers γ and γ^{-1} (as defined in Section 2.3.2) and matrices $X(g)$ and $Y(g)$ which satisfy Eq. (15), the Hilbert space $\mathcal{H}_B$ can be restricted to a representation space of $G \times G$ and thus decomposes into a direct sum of tensor products of irreducible representation spaces of G:*

$$\mathcal{H}_B = \bigoplus_{k=1}^{M} \mathcal{H}_{l_k} \otimes \mathcal{H}_{r_k} ,$$

where r_k and l_k are irreducible representation labels.

Proof. Even though $|\psi_B\rangle$ is defined in terms of the basis $\{|j\rangle\}$ in $\mathcal{H}_B$, it is sufficient to consider only vectors of the form:

$$|\phi_{\alpha,\beta}\rangle = \sum_i \langle\alpha|B^i|\beta\rangle|i\rangle \ \in \mathcal{H}_B .$$

Let $\mathcal{H} := span\{|\phi_{\alpha,\beta}\rangle\}_{\alpha,\beta}$. The group transformations $\mathcal{L}(g)$ and $\mathcal{R}(g)$ preserve $\mathcal{H}$:

$$\mathcal{R}(g)|\phi_{\alpha,\beta}\rangle = \sum_i \langle\alpha|B^iX(g)|\beta\rangle|i\rangle = \sum_{i,\gamma} \langle\alpha|B^i|\gamma\rangle\langle\gamma|X(g)|\beta\rangle|i\rangle = \sum_\gamma \langle\gamma|X(g)|\beta\rangle|\phi_{\alpha,\gamma}\rangle$$

$$\mathcal{L}(g)|\phi_{\alpha,\beta}\rangle = \sum_i \langle\alpha|Y(g)^{-1}B^i|\beta\rangle|i\rangle = \sum_{i,\gamma} \langle\alpha|Y(g)^{-1}|\gamma\rangle\langle\gamma|B^i|\beta\rangle|i\rangle = \sum_\gamma \langle\alpha|Y(g)^{-1}|\gamma\rangle|\phi_{\gamma,\beta}\rangle ,$$

where Eq. (15) was used. Performing a Schmidt decomposition of $|\psi_{AB}\rangle$ (or $|\psi_B\rangle$, the argument is the same) with respect to any partition where one gauge field Hilbert space is split off from the rest of the system:

$$|\psi_{AB}\rangle = \sum_{\{i\},\{j\},\alpha,\beta} \left(\langle\alpha|B^{j_1}|\beta\rangle \ \langle\beta|A^{i_2}B^{j_2}\dots A^{i_N}B^{j_N}A^{i_1}|\alpha\rangle\right) \ |i_1\rangle \otimes |j_1\rangle \otimes |i_2 \dots i_N j_N\rangle$$

$$= \sum_{\alpha,\beta} |\phi_{\alpha,\beta}\rangle_{[2]}|\psi_{\beta,\alpha}\rangle_{[3,\dots,2N,1]} ,$$

we see that only vectors from $\mathcal{H}$ appear. Therefore it is sufficient to restrict ourselves to $\mathcal{H}_B = \mathcal{H}$. Next we show that $\mathcal{H}$ has a representation space structure. Eq. (15) implies that $\mathcal{R}(g)$ and $\mathcal{L}(h)$ commute on $\mathcal{H}$:

$$\mathcal{L}(g)\mathcal{R}(h)|\phi_{\alpha,\beta}\rangle = \sum_i \langle\alpha|Y(g)^{-1}B^iX(h)|\beta\rangle|i\rangle = \mathcal{R}(h)\mathcal{L}(g)|\phi_{\alpha,\beta}\rangle\ .$$

Thus $\mathcal{H}$ forms a projective representation space of $G\times G$ with the projective representation map $(g,h)\mapsto \mathcal{L}(g)\mathcal{R}(h)$ with multiplier $\gamma^{-1}\times\gamma$ of $G\times G$ defined by $\gamma^{-1}\times\gamma\ :\ ((g,h),(g',h'))\mapsto \gamma^{-1}(g,g')\gamma(h,h')$ [42]:

$$\mathcal{L}(g)\mathcal{R}(h)\mathcal{L}(g')\mathcal{R}(h')|_{\mathcal{H}} = \mathcal{L}(g)\mathcal{L}(g')\mathcal{R}(h)\mathcal{R}(h')|_{\mathcal{H}} = \gamma^{-1}(g,g')\gamma(h,h')\mathcal{L}(gg')\mathcal{R}(hh')|_{\mathcal{H}}\ ,$$

where we used the fact that $\mathcal{L}(g)$ and $\mathcal{R}(h)$ commute and preserve $\mathcal{H}$; . For finite or compact groups $\mathcal{H}$ decomposes into a direct sum of irreducible projective representations of $G\times G$ with multiplier $\gamma^{-1}\times\gamma$, each one of which is equivalent to a projective representation of the form $(g,h)\mapsto D^l_{\gamma^{-1}}(g)\otimes D^r_\gamma(h)$ [42], which proves the proposition. □

Recall the definition of an elementary B block:

Definition 3.1. An elementary block of the tensor B is one which satisfies Eq. (15), where $\mathcal{R}(g)=\mathbb{I}\otimes D^r_\gamma(g)$, $\mathcal{L}(g)=D^l_{\gamma^{-1}}(g)\otimes\mathbb{I}$ and $X(g)$, $Y(g)$, $D^r_\gamma(g)$ and $D^l_{\gamma^{-1}}(g)$ are irreducible projective representations (both $X(g)$ and $Y(g)$ have multiplier γ).

Proposition 3 (*Structure of an elementary B block*)**.** *Let B be an elementary B block (Definition 3.1). If $X(g)=D^r_\gamma(g)$ and $\overline{Y(g)}=D^l_{\gamma^{-1}}(g)$, then B is proportional to the tensor composed of the matrices*

$$B^{m,n} = |m\rangle\langle n|\ ,\ m=1,\dots,dim(l),\ n=1,\dots,dim(r)\ .$$

Otherwise $B=0$.

Proof. Write B as a map $B:\mathbb{C}^{D_2}\to\mathbb{C}^{D_1}\otimes\mathcal{H}_B$:

$$B=\sum_{m,n}B^{m,n}\otimes|m\rangle|n\rangle = \sum_{m,n,\alpha,\beta}B^{m,n}_{\alpha,\beta}|\alpha\rangle\langle\beta|\otimes|m\rangle|n\rangle$$

By hypothesis B satisfies (Eq. (15)):

$$[\mathbb{I}\otimes(\mathcal{R}(g)\mathcal{L}(h))]\,B = \left[\mathbb{I}\otimes\left(D^l_{\gamma^{-1}}(h)\otimes D^r_\gamma(g)\right)\right]B = \left[Y(h)^{-1}\otimes\mathbb{I}\right]B\,[X(g)\otimes\mathbb{I}]\ .$$

Write the above equality explicitly (repeated indices are summed over):

$$\begin{aligned}
LHS &= \sum B^{m,n}_{\alpha,\beta}|\alpha\rangle\langle\beta|\otimes D^l_{\gamma^{-1}}(h)|m\rangle D^r_\gamma(g)|n\rangle\\
&= \sum B^{m,n}_{\alpha,\beta}|\alpha\rangle\langle\beta|\otimes D^l_{\gamma^{-1}}(h)_{m',m}|m'\rangle D^r_\gamma(g)_{n',n}|n'\rangle =\\
RHS &= \sum B^{m,n}_{\alpha,\beta}Y(h)^{-1}|\alpha\rangle\langle\beta|X(g)\otimes|m\rangle|n\rangle\\
&= \sum B^{m,n}_{\alpha,\beta}\overline{Y(h)_{\alpha,\alpha'}}|\alpha'\rangle\langle\beta'|X(g)_{\beta,\beta'}\otimes|m\rangle|n\rangle\ .
\end{aligned}$$

Projecting both LHS and RHS to $|\hat\alpha\rangle\langle\hat\beta|\otimes|\hat m\rangle|\hat n\rangle$ we obtain

$$\sum_{m,n}D^l_{\gamma^{-1}}(h)_{\hat m,m}D^r_\gamma(g)_{\hat n,n}B^{m,n}_{\hat\alpha,\hat\beta} = \sum_{\alpha,\beta}B^{\hat m,\hat n}_{\alpha,\beta}\overline{Y(h)_{\alpha,\hat\alpha}}X(g)_{\beta,\hat\beta}\ .$$

The LHS is a multiplication from the left (summing the indices m,n) of the matrix $\mathbf{B}$, with entries $\mathbf{B}_{(m,n),(\alpha,\beta)}:=B^{m,n}_{\alpha,\beta}$, with the matrix $D^l_{\gamma^{-1}}(h)\otimes D^r_\gamma(g)$, which is an irreducible projective representation of $G\times G$. The RHS is a multiplication of $\mathbf{B}$ from the right (summing the indices α,β) with the matrix $\overline{Y(h)}\otimes X(g)$, which is also an irreducible projective representation of $G\times G$ (with the same multiplier).

By Schur's lemma (Lemma 2.1) $\mathbf{B} \propto \mathbb{I}$ (i.e. $B^{m,n}_{\alpha,\beta} \propto \delta_{\alpha,m}\delta_{\beta,n}$) if $D^{l}_{\gamma^{-1}}(h) \otimes D^{r}_{\gamma}(g) = \overline{Y(h)} \otimes X(g)$, and zero otherwise. □

Proposition 4. *Let B, $\mathcal{R}(g)$, $\mathcal{L}(g)$ and $X(g)$ be as in Theorem 2. Let $X_j(g) = \oplus_a X^a_j(g)$ be a block of $X(g)$ appearing in Eq. (14), consisting of irreducible projective representations $X^a_j(g)$. Let $\mathcal{R}(g) = \oplus_k(\mathbb{I}\otimes D^{r_k}_{\gamma}(g))$ and $\mathcal{L}(g) = \oplus_k(D^{l_k}_{\gamma^{-1}}(g) \otimes \mathbb{I})$, where $D^{r_k}_{\gamma}$ and $D^{l_k}_{\gamma^{-1}}$ are irreducible projective representations. Then the following hold:*

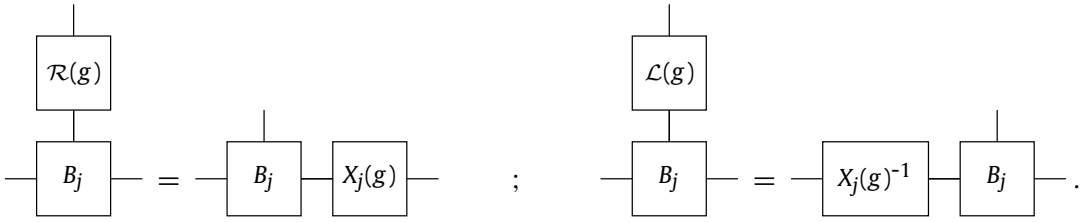
1. *For all k either there exist a and b such that $X^b_j(g) = D^{r_k}_{\gamma}(g)$ and $\overline{X^a_j(g)} = D^{l_k}_{\gamma^{-1}}(g)$, or the projection of the corresponding tensor B_j (a BNT element of B) to the sector k of the physical space is zero.*
2. *$\forall a \ \exists k$ such that $\overline{X^a_j(g)} = D^{l_k}_{\gamma^{-1}}(g)$.*
3. *$\forall a \ \exists k$ such that $X^a_j(g) = D^{r_k}_{\gamma}(g)$.*

Proof. Recall the structure of the tensor B and the projective representation $X(g)$:

$$B^{k;m,n} = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} \mu_{j,q} B^{k;m,n}_j$$

$$X(g) = \oplus_{j=1}^{m} \oplus_{q=1}^{r_j} X_j(g)\,,$$

where $\{B_j\}$ are normal tensors. Project Eq. (13) to a block j, q of the virtual space to obtain:

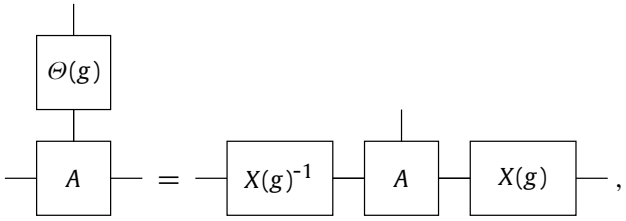


Let $X_j(g) = \oplus_a X^a_j(g)$ be a block of $X(g)$. We shall prove each item in the statement:

1. Let B^k_j be the projection of the tensor B_j to the k sector of the physical Hilbert space. If for a certain k there exist no a and b such that $X^b_j(g) = D^{r_k}_{\gamma}(g)$ and $\overline{X^a_j(g)} = D^{l_k}_{\gamma^{-1}}(g)$, then according to Proposition 3, for all a, b the a, b block of B^k_j, consisting of the matrices $B^{k,m,n}_{j,a,b}$, is zero. This means B^k_j is zero.
2. If there is a $Y^a(g)$ for which there is no appropriate k then according to Proposition 3, $B^{k,m,n}_j$ all have a zero row which is a contradiction to the normality of B_j.
3. As in Item 2, $B^{k,m,n}_j$ now would have a zero column, which contradicts the normality of B_j. □

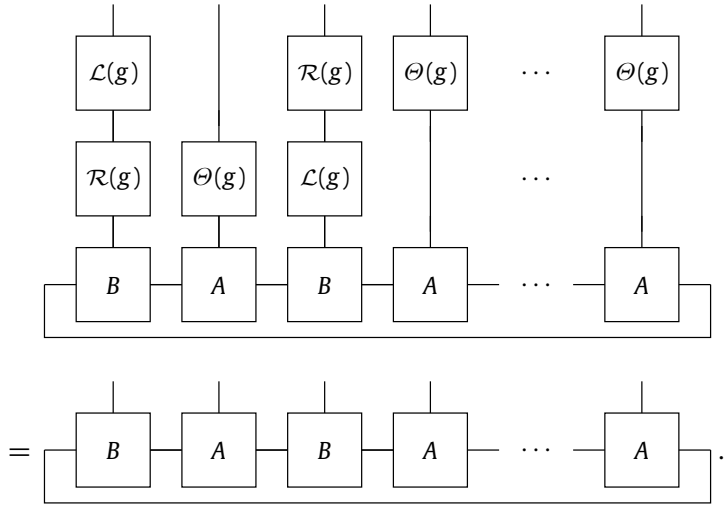
The proof of Proposition 5 will be presented in the next section after we derive the structure of the symmetric matter tensor A.

Proposition 6. *Let B, $\mathcal{R}(g)$ and $\mathcal{L}(g)$ be as in Theorem 2 and in addition let span$\{B^{k;m,n} \mid k, m, n\}$ contain the identity matrix (e.g. Eq. (18)). Let A and $\Theta(g)$ be such that the MPV generated by AB has a local symmetry with respect to $\mathcal{R}(g) \otimes \Theta(g) \otimes \mathcal{L}(g)$ (Definition 4). Then $|\psi^N_A\rangle$ has a global symmetry with respect to $\Theta(g)$. If in addition A is in CF with the same block structure as B (Eq. (12)), then A transforms as:*

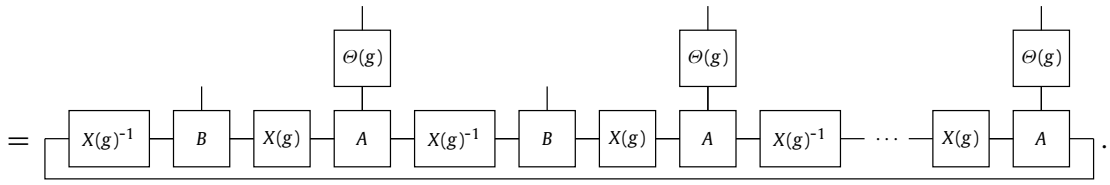


with the same $X(g)$ from Theorem 2.

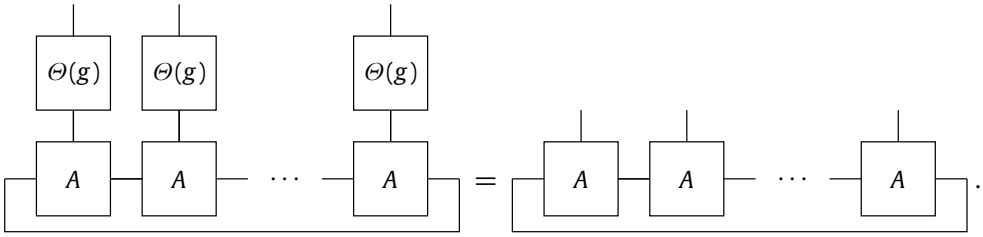
Proof. We use the local symmetry condition around every A:



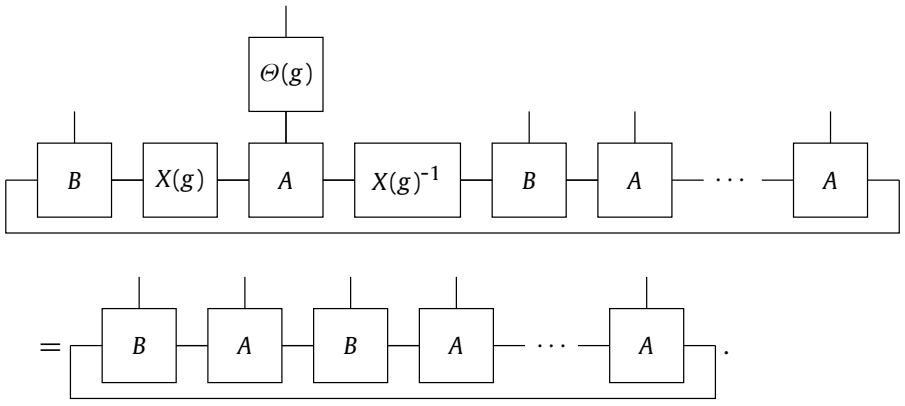
According to the transformation laws for B, the LHS of the above equals:



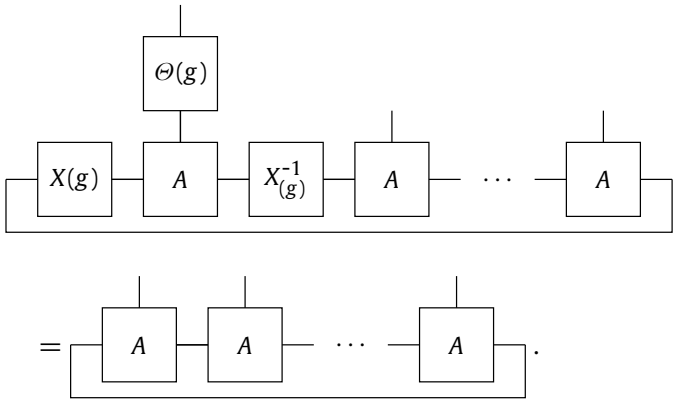
We can now use the assumption $\mathbb{I} \in span\{B^{k;m,n}\}$ to eliminate the Bs from the equation, the Xs then cancel out and we obtain the desired global symmetry:



If in addition A is in CF, we can apply Theorem 4 to obtain transformation relations for A. To show the rest of the claim (if A in addition has the block structure of B) we write the symmetry condition and again use the transformation rules for B:



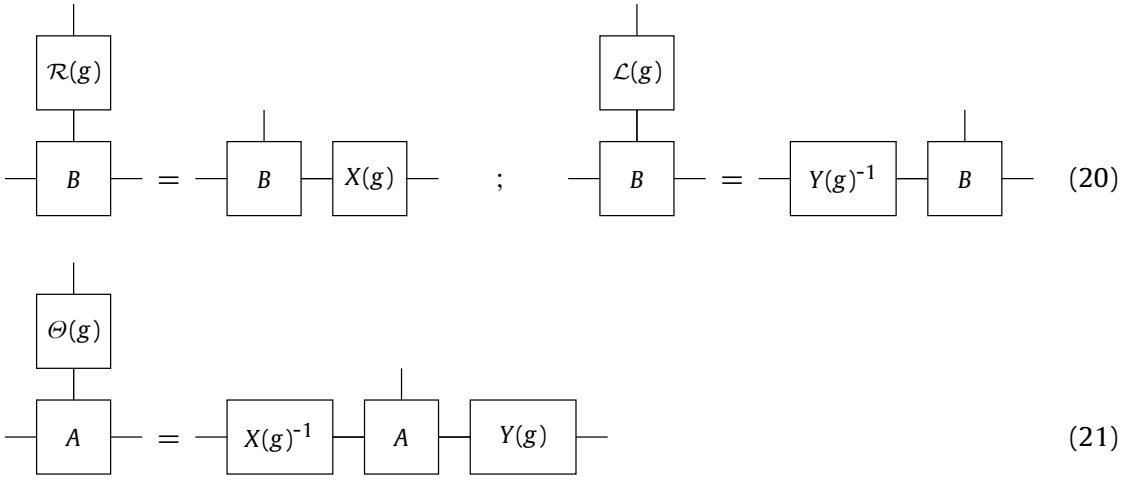
We eliminate all Bs as before and are left with:



We can now use Lemma 4.1 with $S^i = A^i$ and $T^i = X(g)\sum_{i'}\Theta(g)_{ii'}A^{i'}X(g)^{-1}$ to finish the proof (this is where we use the assumption about the block structure of A, the crucial thing is that $X(g)$ is compatible with A's blocks as in Lemma 4.1). □

5.3. Matter and gauge field MPV

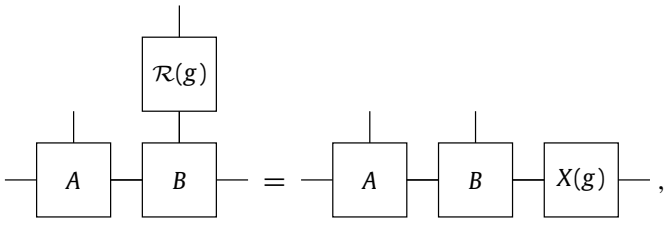
Theorem 3 (*Matter and gauge field MPV with a local symmetry*)**.** *Let both BA and AB be normal tensors in CFII and let $\Theta(g)$ and $\mathcal{R}(g)$, $\mathcal{L}(g)$ be unitary and projective representations (with inverse multipliers) of a group G respectively. Let $|\psi_{AB}^N\rangle$ be a MPV with a local symmetry with respect to $\mathcal{R}(g)\otimes\Theta(g)\otimes\mathcal{L}(g)$ (Definition 4). Then there exist projective representations $X(g)$ and $Y(g)$ on $\mathbb{C}^{D_1}$ and $\mathbb{C}^{D_2}$ respectively, such that $X(g)$ has the same multiplier as $\mathcal{R}(g)$, and $Y(g)$ - the inverse multiplier to that of $\mathcal{L}(g)$. The tensors A and B transform as follows:*



(20)

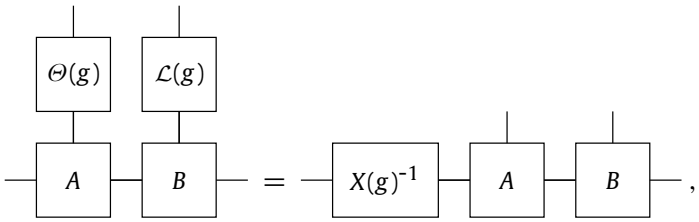
(21)

Proof. Apply Theorem 2 on the tensor AB and the representations $\tilde{\mathcal{R}}(g) := \mathbb{I}\otimes\mathcal{R}(g)$ and $\tilde{\mathcal{L}}(g) := \Theta(g)\otimes\mathcal{L}(g)$ to obtain:



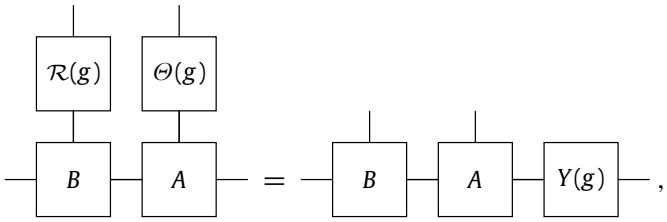
(38)

and



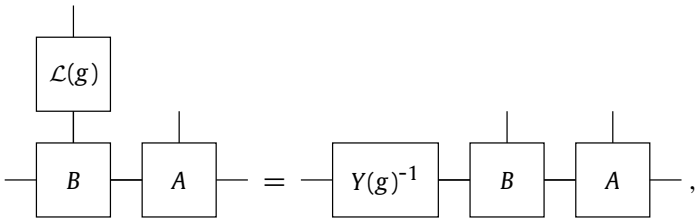
(39)

where $X(g)$ is a projective representation with the same multiplier as $\mathcal{R}(g)$. Apply Theorem 2 once more, this time on the tensor BA and the representations $\tilde{\mathcal{R}}(g) := \mathcal{R}(g) \otimes \Theta(g)$ and $\tilde{\mathcal{L}}(g) := \mathcal{L}(g) \otimes \mathbb{I}$ to obtain:



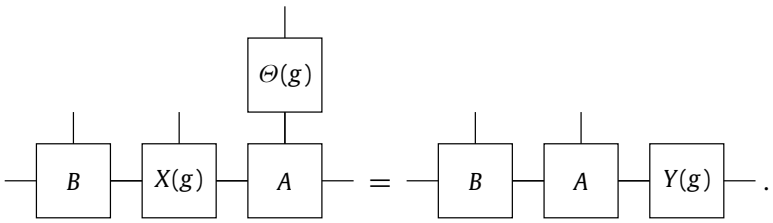
(40)

and



(41)

where $Y(g)$ is a projective representation with inverse multiplier to $\mathcal{L}(g)$. By contracting Eq. (38) from the left with the tensor $BA \ldots B$, and taking the appropriate linear combination to obtain the identity matrix out of the tensor $BA \ldots BA$ (using the normality of BA), we eliminate the A in Eq. (38)). By contracting Eq. (41) with $BA \ldots B$ from the right — we eliminate the A in Eq. (41) (using the normality of AB). This proves the transformation rule for B - Eq. (20). Next plug in the transformation rules of B under $\mathcal{R}(g)$ into Eq. (40) to obtain:



(42)

Finally, eliminate the B from the equation as in the previous steps to obtain the transformation rule for A and finish the proof. □

Proposition 7. *Let $|\psi^N_{AB}\rangle$ be a MPV generated by arbitrary tensors A and B. Then there exist tensors $\{A_\chi\}$ and $\{B_\chi\}$, and there exists $b \in \mathbb{N}$ such that for all χ both $A_\chi B_\chi$ and $B_\chi A_\chi$ are normal tensors and $\forall N \in \mathbb{N}$ $|\psi^N_{AB_{\times b}}\rangle = \sum_\chi \mu^N_\chi |\psi^N_{A_\chi B_\chi}\rangle$, where μ_χ are constants and $AB_{\times b}$ is the tensor obtained by blocking b copies of the tensor AB.*

Proof. We argue similarly to [38] where it is described how to obtain, from an arbitrary tensor, a tensor in CF generating the same MPV. Begin by finding all of AB's minimal invariant subspaces S_α, such that $A^i B^j P_\alpha = P_\alpha A^i B^j P_\alpha$ for all i and j, where P_α is the orthogonal projection to S_α. Let $\hat{P}_\alpha$ be the partial isometry $\hat{P}_\alpha : \mathbb{C}^{D_1} \to S_\alpha$ such that $\hat{P}^\dagger_\alpha \hat{P}_\alpha = P_\alpha$ and $\hat{P}_\alpha \hat{P}^\dagger_\alpha = \mathbb{I}|_{S_\alpha}$. Define $A^i_\alpha := \hat{P}_\alpha A^i$ and

$B^j_\alpha := B^j \hat{P}^\dagger_\alpha$. Then

$$\begin{aligned}
|\psi^N_{AB}\rangle &= \sum_{\{i\},\{j\}} \mathrm{Tr}\left(A^{i_1}B^{j_1}\ldots A^{i_N}B^{j_N}\right)|i_1 j_1\ldots i_N j_N\rangle \\
&= \sum_{\{i\},\{j\},\alpha} \mathrm{Tr}\left(P_\alpha A^{i_1}B^{j_1}\ldots A^{i_N}B^{j_N}P_\alpha\right)|i_1 j_1\ldots i_N j_N\rangle \\
&= \sum_{\{i\},\{j\},\alpha} \mathrm{Tr}\left(P_\alpha A^{i_1}B^{j_1}P_\alpha\ldots P_\alpha A^{i_N}B^{j_N}P_\alpha\right)|i_1 j_1\ldots i_N j_N\rangle \\
&= \sum_{\{i\},\{j\},\alpha} \mathrm{Tr}\left(\hat{P}_\alpha A^{i_1}B^{j_1}\hat{P}^\dagger_\alpha\hat{P}_\alpha\ldots\hat{P}^\dagger_\alpha\hat{P}_\alpha A^{i_N}B^{j_N}\hat{P}^\dagger_\alpha\right)|i_1 j_1\ldots i_N j_N\rangle \\
&= \sum_\alpha |\psi^N_{A_\alpha B_\alpha}\rangle\ .
\end{aligned}$$

Note that the bond dimension of the tensor $A_\alpha B_\alpha$ is $dim(S_\alpha)$ which is smaller than the original bond dimension D_2. Now $A_\alpha B_\alpha$ has no invariant subspaces but $B_\alpha A_\alpha$ might, therefore, perform the same for $B_\alpha A_\alpha$ - for each α find all minimal invariant subspaces $T_{\alpha\beta}$ of $B_\alpha A_\alpha$. Let $Q_{\alpha\beta}$ be the orthogonal projections to the invariant subspaces and $\hat{Q}_{\alpha\beta}$ the partial isometries. Define $A^i_{\alpha\beta} := A^i_\alpha \hat{Q}^\dagger_{\alpha\beta} = \hat{P}_\alpha A^i \hat{Q}^\dagger_{\alpha\beta}$, and $B^j_{\alpha\beta} := \hat{Q}_{\alpha\beta} B^j_\alpha = \hat{Q}_{\alpha\beta} B^j \hat{P}^\dagger_\alpha$. For each α we have

$$|\psi^N_{A_\alpha B_\alpha}\rangle = \sum_\beta |\psi^N_{A_{\alpha\beta} B_{\alpha\beta}}\rangle\ ,$$

and thus

$$|\psi^N_{AB}\rangle = \sum_\alpha |\psi^N_{A_\alpha B_\alpha}\rangle = \sum_{\alpha\beta} |\psi^N_{A_{\alpha\beta} B_{\alpha\beta}}\rangle\ .$$

Now each $A_{\alpha\beta}B_{\alpha\beta}$ might be reducible. Continue iterating this decomposition, once for AB and once for BA. Since the bond dimension of the tensors obtained at each step decreases, this procedure is bound to end after a finite number of steps. In the final step, we obtain the tensors $A^i_\chi = \hat{P}_\chi A^i \hat{Q}^\dagger_\chi$ and $B^j_\chi = \hat{Q}_\chi B^j \hat{P}^\dagger_\chi$, where χ incorporates all the previous indices, such that both $A_\chi B_\chi$ and $B_\chi A_\chi$ have no non trivial invariant subspaces. We can then perform the second step (as in [38]) which involves blocking the tensors in order to eliminate the periodicity of the associated CP maps. The blocking scheme is the following: $\tilde{A}^{ijk} := A^i B^j A^k$ and $\tilde{B}^{lmn} := B^l A^m B^n$. We can find the least common multiple of the length needed to eliminate the periodicity of all CP maps, and perform step 1 again if needed (after blocking the CP maps again become reducible [39]). We can repeat these steps as many times as needed. The process terminates at some point because the bond dimension decreases at each step. Finally, rescale the matrices $A_\chi B_\chi$ by a constant μ_χ to make the spectral radius of $E_{A_\chi B_\chi}$ and $E_{B_\chi A_\chi}$ equal to 1. The following lemma is required:

Lemma 5.2. *$E_{A_\chi B_\chi}$ and $E_{B_\chi A_\chi}$ have the same spectral radius.*

Proof. Let X be an eigenvector of $E_{A_\chi B_\chi}$ with eigenvalue λ: $E_{A_\chi B_\chi}(X) = E_{A_\chi}E_{B_\chi}(X) = \lambda X$. Apply E_{B_χ} to both sides to obtain $E_{B_\chi A_\chi}E_{B_\chi}(X) = \lambda E_{B_\chi}(X)$, i.e., $E_{B_\chi}(X)$ is an eigenvector of $E_{B_\chi A_\chi}$ with eigenvalue λ. Interchanging A and B we obtain that $E_{A_\chi B_\chi}$ and $E_{B_\chi A_\chi}$ have the same spectrum, and therefore the same spectral radius. □

Remark 5.2 (*Blocking of the Symmetry Operators*)**.** In the blocking scheme described in Proposition 7, if we start out with a MPV with a local symmetry under the operators $\mathcal{R}(g)\otimes\Theta(g)\otimes\mathcal{L}(g)$, after blocking we need to redefine the operators to act on the blocked degrees of freedom as follows: $\tilde{\mathcal{R}}(g) := \mathcal{R}(g)\otimes\Theta(g)\otimes(\mathcal{L}(g)\mathcal{R}(g))$, $\tilde{\Theta}(g) := \Theta(g)\otimes(\mathcal{L}(g)\mathcal{R}(g))\otimes\Theta(g)$ and $\tilde{\mathcal{L}}(g) := (\mathcal{L}(g)\mathcal{R}(g))\otimes\Theta(g)\otimes\mathcal{L}(g)$.

Proposition 8. *Let* $|\psi^N_{AB}\rangle = \sum_\chi \mu^N_\chi |\psi^N_{A_\chi B_\chi}\rangle$ *where both* $A_\chi B_\chi$ *and* $B_\chi A_\chi$ *are normal tensors. Let* O *be a local operator acting on a fixed number of adjacent sites. If* $\forall N$ O *leaves the MPV invariant:*

$$O \otimes \mathbb{I}|_{rest} |\psi^N_{AB}\rangle = |\psi^N_{AB}\rangle \ ,$$

then O *leaves every component invariant:*

$$O \otimes \mathbb{I}|_{rest} |\psi^N_{A_\chi B_\chi}\rangle = |\psi^N_{A_\chi B_\chi}\rangle \ \forall \chi \ .$$

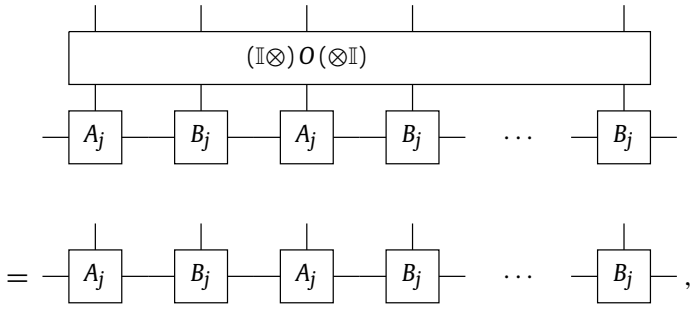
Proof. Pick a BNT $\{A_j B_j\}$ out of the normal tensors $\{A_\chi B_\chi\}$ and construct a new tensor C by blocking the tensors $\{A_\chi B_\chi\}$ diagonally (possibly changing the order of the blocks):

$$C^{ii'} = \oplus_\chi \mu_\chi A^i_\chi B^{i'}_\chi = \oplus_j \oplus_q \mu_{j,q} V^{-1}_{j,q} A^i_j B^{i'}_j V_{j,q} \ ,$$

where for every χ there is a j and a q such that $\mu_\chi A_\chi B_\chi = \mu_{j,q} V^{-1}_{j,q} A^i_j B^{i'}_j V_{j,q}$. Now C is in CF and generates the same MPV as AB. We have

$$O|\psi^N_C\rangle = O|\psi^N_{AB}\rangle = |\psi^N_{AB}\rangle = |\psi^N_C\rangle \ .$$

We can now use Lemma 4.1 (use Eq. (27) from the proof of the lemma) for the tensor $C = AB$ to obtain



where the operator in the box contains O (we need to extend it by at most one $\otimes\mathbb{I}$ from the right and from the left in order to occupy a full $AB \ldots AB$ block). Finally, we have

$$O|\psi^N_{A_\chi B_\chi}\rangle = O|\psi^N_{V^{-1}_{j,q} A_j B_j V_{j,q}}\rangle = |\psi^N_{A_j B_j}\rangle = |\psi^N_{A_\chi B_\chi}\rangle \quad \square$$

Recall the definition of an elementary A block:

Definition 3.2 (*Elementary A Block*)**.** An elementary block of the tensor A is one which satisfies Eq. (21), where $\Theta(g)$, $X(g)$ and $Y(g)$ are all irreducible projective representations.

Proposition 9. *Let* A *be an elementary block (Definition 3.2), with* $\Theta(g) = D^{j_0}(g)$, $X(g) = D^j_\gamma(g)$ *and* $Y(g) = D^l_{\gamma^{-1}}(g)$*. Then* A *is built out of Clebsch–Gordan coefficients and has the form:*

$$A^M = \sum_{J \in \mathfrak{J}: D^J = D^{j_0}} \alpha_J \sum_{m,n} \left\langle J, M \mid \bar{j}, m; l, n \right\rangle |m\rangle\langle n| \ ,$$

where $\mathfrak{J}$ *is the set of irreducible representation indices appearing in the decomposition of* $\overline{D^j_\gamma(g)} \otimes D^l_{\gamma^{-1}}(g)$ *into irreducible representations,* $\left\langle \bar{j}, m : l, n \mid J, M \right\rangle$ *are the Clebsch–Gordan coefficients of the decomposition,* $\overline{D^j_\gamma(g)}$ *is the complex conjugate representation to* $D^j_\gamma(g)$ *and* α_J *are arbitrary constants.*

Proof. Write out Eq. (21):

$$\sum_{i'} \Theta(g)_{ii'} A^{i'} = X(g)^{-1} A^i Y(g) \ .$$

Taking the complex conjugate of both sides

$$\sum_{i'} \Theta(g^{-1})_{i'i} \overline{A^{i'}} = \overline{X(g)^{-1} A^i Y(g)}$$

we see that $\vec{\bar{A}}$ satisfies Eq. (7) for $\vec{v} = \vec{e^i}$ and the group element g^{-1}, with $\kappa = \Theta(g), \pi = \overline{X(g)}$ and $\eta = \overline{Y(g)}$. Therefore $\bar{A}$ is a vector operator with respect to the above representations. In the case when $\Theta(g) = D^{j_0}(g), X(g) = D^j_\gamma(g)$ and $Y(g) = D^l_{\gamma^{-1}}(g)$ are irreducible representations, according to Theorem 2.1 $\bar{A}$ is of the form:

$$\overline{A^M} = \sum_{J:D^j(g)=D^{J_0}(g)} \alpha_J \sum_{m,n} \left\langle \bar{j}, m; l, n \mid J, M \right\rangle |m\rangle\langle n| \,,$$

taking the complex conjugate, we find the desired form of A. □

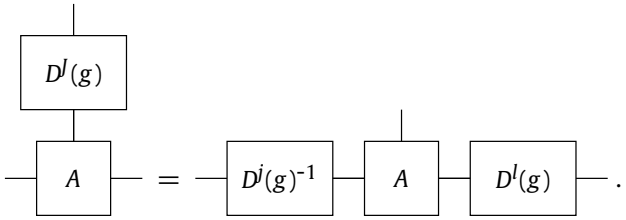
Example 5.1. A direct calculation using the Clebsch–Gordan series [43]:

$$D^j(g)_{m,m'} D^l(g)_{n,n'} = \sum_{L,N,N'} \langle j, m; l, n \mid L, N\rangle \left\langle L, N' \mid j, m'; l, n' \right\rangle D^l(g)_{N,N'}$$

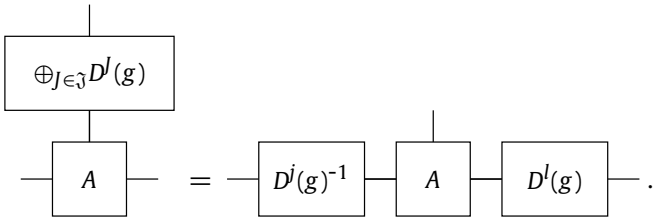
shows that the tensor composed of the matrices

$$A^{J,M} = \sum_{m,n} \left\langle J, M \mid \bar{j}, m; l, n \right\rangle |m\rangle\langle n| \,,$$

for a fixed value of J, satisfies



Consequently, the tensor composed out of all matrices $\{A^{J,M}\}_{J\in\mathfrak{J},M}$ (all J appearing in the decomposition $\overline{D^j(g)} \otimes D^l(g) = \oplus_{J\in\mathfrak{J}} D^J(g)$) satisfies:



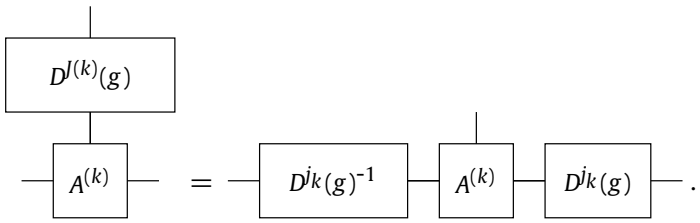
In addition to being a symmetric tensor, this tensor is always injective: let $D := dim(j) = dim(l)$. Due to the fact that the C–G coefficients are the entries of a unitary matrix, the matrices $A^{J,M}$ satisfy $\mathrm{Tr}\left(A^{J,M\,\dagger} A^{J',M'}\right) = \delta_{J,J'}\delta_{M,M'}$. Since there are $D \times D$ of them, they form an ONB of the space of $D \times D$ matrices.

We can now prove the following proposition, the proof of which we postponed in the previous section.

Proposition 5. *Let B be in CFII and let $|\psi_B^N\rangle$ have a local symmetry with respect to $\mathcal{R}(g) \otimes \mathcal{L}(g)$ (as in Theorem 2). It is always possible to find a tensor A and a representation $\Theta(g)$ such that the corresponding matter and gauge field MPV $|\psi_{AB}^N\rangle$ has a local symmetry with respect to $\mathcal{R}(g) \otimes \Theta(g) \otimes \mathcal{L}(g)$ (Definition 4). In addition, the corresponding matter MPV - $|\psi_A^N\rangle$ - has a global symmetry with respect to $\Theta(g)$.*

Proof. For each $D^{j_k}_\gamma(g)$ appearing in $\underline{X(g)} = \oplus_{k=1}^s D^{j_k}_\gamma(g)$, let $J(k)$ be an irreducible representation index appearing in the decomposition of $\overline{D^{j_k}_\gamma(g)} \otimes D^{j_k}_\gamma(g)$. Let $A^{(k)}$ be the tensor presented in Example 5.1,

satisfying



Let the matter Hilbert space be $\mathcal{H}_A := \oplus_k \mathcal{H}_{J(k)}$. Let the tensor A in each sector $J(k)$ of the physical space be zero except for in the k, k virtual block, such that:

$$\left[X^{-1}(g)A^{j_k,M}X(g)\right]_{l,l'} = \delta(l,k)\delta(l',k)D^{j_k}_{M,M'}(g)A^{(k)j_k,M'} \,. \quad \square$$

Proposition 10. *Let AB and BA be normal tensors and let B satisfy Eq. (20) with $\mathcal{R}(g) = \oplus_k(\mathbb{I} \otimes D^{r_k}_{\gamma}(g))$, $\mathcal{L}(g) = \oplus_k(D^{l_k}_{\gamma^{-1}}(g)\otimes\mathbb{I})$, $Y(g) = \oplus_a Y^a(g)$ and $X(g) = \oplus_b X^b(g)$, where $D^{r_k}_{\gamma}$, $D^{l_k}_{\gamma^{-1}}$, Y^a and X^b are irreducible projective representations, then*

1. *For all k either there exist a and b such that $X^b(g) = D^{r_k}_{\gamma}(g)$ and $\overline{Y^a(g)} = D^{l_k}_{\gamma^{-1}}(g)$ or the projection of the tensor B to the sector k of the physical space is zero (and it can be discarded).*
2. *$\forall a$ $\exists k$ such that $\overline{Y^a(g)} = D^{l_k}_{\gamma^{-1}}(g)$.*
3. *$\forall b$ $\exists k$ such that $X^b(g) = D^{r_k}_{\gamma}(g)$.*

Proof.

1. Assume the contrary is true, then according to Proposition 3, $B^{k,m,n}$ are all zero and this value of k does not contribute to the MPV.
2. If there is a $Y^a(g)$ for which there is not an appropriate k then according to Proposition 3, $B^{k,m,n}$ all have a zero row which is a contradiction to the normality of AB.
3. As in Item 2, $B^{k,m,n}$ now would have a zero column and would contradict normality of BA. $\square$

Proposition 11. *There exist tensors A and B such that $|\psi_{AB}\rangle$ has a local symmetry with respect to $\mathcal{R}(g) \otimes \Theta(g) \otimes \mathcal{L}(g)$, but $|\psi_A\rangle$ does not have a global symmetry with respect to $\Theta(g)$. In addition $\mathcal{R}(g) \otimes \mathcal{L}(g)|\psi_B\rangle \neq |\psi_B\rangle$.*

The proof is given by the following example:

Example 5.2. Let $G = D_{10}$ the dihedral group of order 10. It is the group generated by two elements: r and s satisfying $r^5 = s^2 = (sr)^2 = e$. D_{10} has two inequivalent two dimensional irreducible representations ρ_1 and ρ_2 generated by:

$$\rho_1 : r \mapsto R_1 := \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}$$

$$s \mapsto S := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\rho_2 : r \mapsto R_2 := \begin{pmatrix} e^{i2\theta} & 0 \\ 0 & e^{-i2\theta} \end{pmatrix}$$

$$s \mapsto S := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

where $\theta = 2\pi/5$. The tensor product $\overline{\rho_1} \otimes \rho_2$ decomposes into $\rho_1 \oplus \rho_2$:

$$\overline{\rho_1} \otimes \rho_2 : r \mapsto R_1 \otimes R_2 = \begin{pmatrix} e^{i\theta} & 0 & 0 & 0 \\ 0 & e^{-i3\theta} & 0 & 0 \\ 0 & 0 & e^{i3\theta} & 0 \\ 0 & 0 & 0 & e^{-i\theta} \end{pmatrix}$$

$$s \mapsto S \otimes S = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} .$$

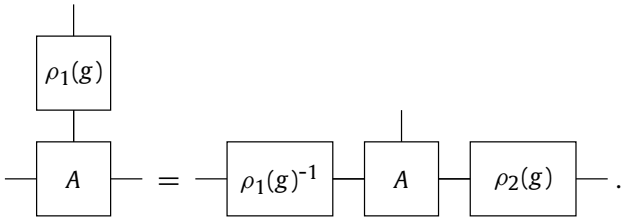
It is clear from inspection of the above 4×4 matrices that the unitary transformation realizing the direct sum decomposition is a permutation of the basis elements, the non zero Clebsch–Gordan coefficients are:

$$\langle \rho_1, 1 \,|\, \overline{\rho_1}, 1; \rho_2, 1\rangle = 1$$
$$\langle \rho_1, 2 \,|\, \overline{\rho_1}, 2; \rho_2, 2\rangle = 1$$
$$\langle \rho_2, 1 \,|\, \overline{\rho_1}, 1; \rho_2, 2\rangle = 1$$
$$\langle \rho_2, 2 \,|\, \overline{\rho_1}, 2; \rho_2, 1\rangle = 1 .$$

Following Example 5.1, and using these coefficients, define the tensor A:

$$A^1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad A^2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} .$$

A satisfies:

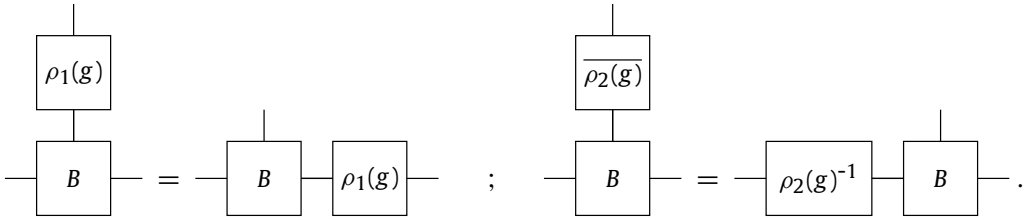


(43)

According to Proposition 3 the following tensor B:

$$B^{1,1} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad B^{1,2} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$
$$B^{2,1} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad B^{2,2} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} ,$$

satisfies:



(44)

Eqs. (43) and (44) are easily verified for the generators of the group, r and s, and therefore hold for any group element. From these equations it follows that $|\psi^N_{AB}\rangle$ has a local symmetry (Definition 4 with $\mathcal{R}(g) = \rho_1(g)$, $\Theta(g) = \rho_1(g)$ and $\mathcal{L}(g) = \overline{\rho_2(g)}$); however, ρ_1 is not a global symmetry for $|\psi^N_A\rangle$, as is easily verified for a MPV of length 1. Similarly, a direct computation shows $\mathcal{R}(g) \otimes \mathcal{L}(g)|\psi^2_B\rangle \neq |\psi^2_B\rangle$.

Proposition 12. *Let A be a tensor in CFII generating a MPV with a global symmetry i.e., satisfying Theorem 4. Let $X(g)$ (in Eq. (23)) be a projective representation (i.e. all $X_j(g)$ in Eq. (24) are in the same cohomology class). Then there exist a tensor B and projective representations $\mathcal{R}(g)$ and $\mathcal{L}(g)$ with inverse multipliers such that both local symmetries: Definition 4 for $|\psi_{AB}^N\rangle$ and Definition 3 for $|\psi_B^N\rangle$ are satisfied.*

Proof. As $X(g)$ appears in Eq. (23) together with its inverse, it is defined only up to a phase. As we assumed all $X_j(g)$ are from the same cohomology class, we can lift each one of them to be projective representations with the same multiplier γ. We can assume without loss of generality (same argument as in Remark 3.3) that each $X_j(g)$ is block diagonal: $X(g) = \oplus_j \oplus_q \oplus_{a_j} D_\gamma^{a_j}(g)$. Set $\mathcal{R}(g) = X(g)$, $\mathcal{L}(g) = \overline{X(g)}$ and let B be completely block diagonal:

$$B^{j,q,a_j;m,n} = |j, q, a_j; m\rangle\langle j, q, a_j; n| \,,$$

i.e., for each irreducible block of $X(g)$ there is a corresponding sector in $\mathcal{H}_B$:

$$\mathcal{H}_B = \oplus_j \oplus_q \oplus_{a_j} \mathcal{H}_{\overline{a_j}} \otimes \mathcal{H}_{a_j} \,,$$

where $\overline{a_j}$ is the complex conjugate representation to a_j. □

Example 5.3 (*An $SU(2)$ Gauge Invariant MPV*)**.** For $G = SU(2)$ we demonstrate the construction of a general locally invariant MPV emphasizing the constituents of physical theories and relating our setting and notation to [34,36]. Write the irreducible representations $D^j(g)$ in terms of their generators:

$$D^j(g) = \exp\left(i \sum_a \tau_a^j \varphi_a(g)\right), \ \forall g \in SU(2),$$

where $\{\varphi_a(g)\}_{a=1}^3$ are real parameters and $\{\tau_a^j\}_{a=1}^3$ are Hermitian $(2j+1)\times(2j+1)$ matrices satisfying the $\mathfrak{su}(2)$ Lie algebra relations:

$$\left[\tau_a^j, \tau_b^j\right] = i\varepsilon_{abc}\tau_c^j \,,$$

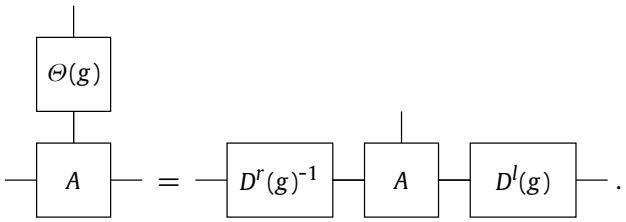
where ε_{abc} is the totally antisymmetric tensor. Let D^r and D^l be two irreducible representations of $SU(2)$ and let $\mathfrak{J}_0$ be the set of irreducible representation indices appearing in the decomposition of the tensor product: $\overline{D^r(g)} \otimes D^l(g) \cong \oplus_{J\in\mathfrak{J}_0} D^J(g)$. Let $\mathfrak{J} \subseteq \mathfrak{J}_0$. Define the representation $\Theta(g)$ as generated by $\{Q_a := \oplus_{J\in\mathfrak{J}} \tau_a^J\}_{a=1}^3$:

$$\Theta(g) = \oplus_{J\in\mathfrak{J}} D^J(g) = \oplus_{J\in\mathfrak{J}} \exp\left(i \sum_a \tau_a^J \varphi_a(g)\right) = \exp\left(i \sum_a Q_a \varphi_a(g)\right) \,.$$

As in Example 5.1, the tensor A, defined by the matrices:

$$A^{J,M} = \sum_{m,n} \alpha_J \, \langle J, M \mid \bar{r}, m; l, n\rangle \, |m\rangle\langle n| \,, J \in \mathfrak{J}, M = 1, \ldots, dim(J) \tag{45}$$

satisfies:



This relation, written in terms of the generators, reads:

$$\sum_{M'}\left[\exp\left(i\sum_a \tau_a^J\varphi_a(g)\right)\right]_{M,M'} A^{J,M'} = \exp\left(-i\sum_a \tau_a^r\varphi_a(g)\right) A^{J,M} \exp\left(i\sum_a \tau_a^l\varphi_a(g)\right) .$$

Differentiating this equation with respect to any one of the group parameters φ_a we obtain the "virtual Gauss law" satisfied by A:

$$Q_a : A^{J,M} \mapsto \sum_{M'} \left[\tau_a^J\right]_{M,M'} A^{J,M'} = -\tau_a^r A^{J,M} + A^{J,M}\tau_a^l .$$

Next, add a gauge field degree of freedom to the matter MPV, described by a tensor: $B^{m,n} = |m\rangle\langle n|$, and define the transformations:

$$\mathcal{R}(g) = \mathbb{I} \otimes D^r(g) \quad ; \quad \mathcal{L}(g) = \overline{D^l(g)} \otimes \mathbb{I} .$$

The action of $\mathcal{L}(g)$ on the gauge field Hilbert space is given by:

$$\mathcal{L}(g)|m,n\rangle = (\overline{D^l(g)} \otimes \mathbb{I})|m,n\rangle = \sum_{m'} \overline{D^l(g)}_{m',m}|m',n\rangle = \sum_{m'} D^l(g^{-1})_{m,m'}|m',n\rangle ;$$

whereas $\mathcal{R}(g)$ acts as:

$$\mathcal{R}(g)|m,n\rangle = \sum_{n'} D^r(g)_{n',n}|m,n'\rangle .$$

$\mathcal{R}(g)$ and $\mathcal{L}(g)$ can be defined in terms of right and left generators $\{R_a\}_{a=1}^3$ and $\{L_a\}_{a=1}^3$, as described in Section 2.4:

$$\mathcal{R}(g) = \exp\left(i\sum_a R_a\varphi_a(g)\right)$$

$$\mathcal{L}(g) = \exp\left(i\sum_a L_a\varphi_a(g)\right) .$$

In our case R_a is simply given by $\mathbb{I} \otimes \tau_a^r$ but in general R_a and L_a can have a block diagonal structure. Define the generators of the local gauge transformation around lattice site $2K+1$:

$$G_a^{[2K+1]} := \left(R_a^{[2K]} + Q_a^{[2K+1]} + L_a^{[2K+2]}\right) .$$

From our construction it follows that for all $g \in G$ and for all lattice sites K:

$$\mathcal{R}^{[2K]}(g) \otimes \Theta^{[2K+1]}(g) \otimes \mathcal{L}^{[2K+2]}(g)|\psi_{AB}^N\rangle = |\psi_{AB}^N\rangle .$$

Once again, differentiating with respect to the group parameters φ_a we obtain:

$$\left(R_a^{[2K]} + Q_a^{[2K+1]} + L_a^{[2K+2]}\right)|\psi_{AB}^N\rangle = G_a^{[2K+1]}|\psi_{AB}^N\rangle = 0 . \tag{46}$$

This is the lattice version of Gauss' law. In physical theories $D^l = \overline{D^r}$ and thus states $|\psi_A\rangle$ have a global symmetry generated by $\{Q_a\}$ - the $SU(2)$ charge operators. R_a and L_a are identified with right and left electric fields respectively [36].

One could generalize the above construction for

$$\mathcal{R}(g) = \oplus_k \left(\mathbb{I} \otimes D^{r_k}(g)\right) \quad ; \quad \mathcal{L}(g) = \oplus_k \left(\overline{D^{l_k}(g)} \otimes \mathbb{I}\right)$$

by constructing A and B as above for each k sector and combining them together block diagonally (in both physical and virtual dimensions). Duplicating the virtual representations while keeping the physical ones fixed can be achieved by $B^{m,n} \mapsto (B^{m,n} \oplus B^{m,n})$, $A^{J,M} \mapsto (A_1^{J,M} \oplus A_2^{J,M})$. This can be used to enlarge the number of variational parameters. The tensors A_1 and A_2 must both have the same structure (Eq. (45)) but can have different parameters α_J. The generalization to of the above to $G = SU(N)$ is straightforward.

6. Summary

In this work, we studied and classified translationally invariant MPVs with a local (gauge) symmetry under arbitrary groups. The states we classified may involve two types of building blocks, A and B tensors, which represent matter and gauge fields respectively.

We showed that matter-only MPVs may have a local symmetry, when one transforms a single site, only if they are trivial (composed of products of invariant states at each site). We also classified pure gauge states, which involve only B tensors and have local invariance when one transforms two neighboring sites, including the well-known structure of physical states involving only gauge fields. These two building blocks can be combined in a way that allows coupling matter fields (with global symmetry) to gauge fields (with local symmetry) in a locally symmetric manner, as in conventional gauge theory scenarios. Furthermore, we expanded the class of gauge invariant states to include ones that involve matter and gauge fields which do not possess the known symmetry properties when decoupled. We classified the structure and properties of such MPVs as well.

Further work shall include a generalization to further dimensions, i.e. using PEPS. In our work we were able to connect some of the results to the symmetry properties and structure of previous gauge invariant PEPS constructions [31,32,34] when the space dimension is reduced to one, and therefore higher dimensional generalizations in the spirit of the current work should be possible. In particular, the tensor describing the gauge field, as it resides on the links of a lattice, is a one dimensional object for any spatial dimension, and has shown, in some particular cases, properties known from previous PEPS studies. Another important generalization one should consider is a fermionic representation of the matter, combining the spirit of this work with previous works on fermionic PEPS with gauge symmetry [33,35] or with global symmetry [50,51]. From the physical point of view, a physical study aiming at understanding the new classes of gauge invariant states introduced in this paper, in which the matter and gauge field do not possess separate symmetries, may also potentially unfold new physical phenomena and phases.

Acknowledgment

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3.5 Normal tensors generating the same state

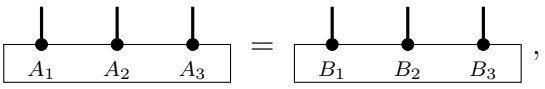
In this Section, we include the following paper:

- Andras Molnar, José Garre-Rubio, David Pérez- García, Norbert Schuch, and J. Ignacio Cirac. "Normal projected entangled pair states generating the same state". In: *New J. Phys.* 20, 113017 (Nov. 2018), p. 113017. arXiv: 1804.04964

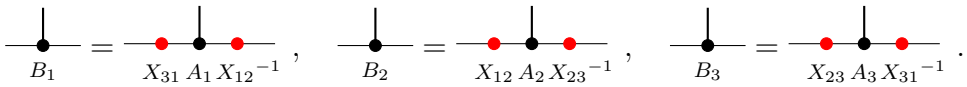
In the previous projects the ability of deciding when two TNS generate the same state played a crucial role. Due to their importance, theorems deciding this question are often referred to as fundamental theorems. In Section 3.3, the use of two such different theorems lead to the classification of 2D SPT phases: first, we had to decide whew two semi-injective tensor generate the same state; second, for classifying MPO representations we had to decide when a general MPS tensor generates the same state as an injective tensor. In Section 3.4 the investigation of local symmetries required a version of the fundamental theorem with non-TI tensors. There are several other examples for using such fundamental theorems including the classification of Matrix Product Unitaries with and without symmetries [72, 73] as well as the classification of renormalization fixed points of Matrix Product Density Operators [52].

In this project, we prove the fundamental theorem for non-translationally invariant PEPS for arbitrary lattice geometry provided that the generating tensors are normal. This question thus encompasses the investigation of local symmetries by allowing for non-translationally invariant description of the states. It also generalizes the results of Ref. [67] as it holds in arbitrary dimensions or non-square lattice geometry such as hyperbolic lattices relevant in the constructions of AdS/CFT correspondence [74, 75].

We find that despite the non-translational description, if two sets of normal tensors generate the same state, the tensors are related to each other with local, invertible operators acting on the virtual indices. These gauges can depend on the bond; for example, two three-partite non-translationally invariant injective MPS generates the same state:



if and only if there are invertible operators X_{12}, X_{23} and X_{31} such that the generating tensors A_i and B_i are related to each other as



In fact, this statement is the basic lemma of the paper, all other normal tensor networks can be blocked into three-partite injective MPS determining the gauge transformation assigned to a given bond.

This project was later used to classify entanglement properties of MPS (Section 3.7). This is possible as the theorem allows for comparing two non-TI MPS and thus general

non-TI SLOCC transformations can be analyzed. While the main theorem is more general than the previous such theorems, the conditions under which one can use the theorem are still restrictive: both sets of tensors have to be normal. It is natural to ask how this can be generalized. In the next Section, we show that one should not expect to be able to decide whether two arbitrary PEPS tensors generate the same stat.

Normal projected entangled pair states generating the same state

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Tensor networks are generated by a set of small rank tensors and define many-body quantum states in a succinct form. The corresponding map is not one-to-one: different sets of tensors may generate the very same state. A fundamental question in the study of tensor networks naturally arises: what is then the relation between those sets? The answer to this question in one dimensional setups has found several applications, like the characterization of local and global symmetries, the classification of phases of matter and unitary evolutions, or the determination of the fixed points of renormalization procedures. Here we answer this question for projected entangled-pair states (PEPS) in any dimension and lattice geometry, as long as the tensors generating the states are normal, which constitute an important and generic class.

I. INTRODUCTION

Tensor Networks (TNs) provide us with very efficient ways of describing quantum states in discrete systems. They are particularly useful to describe ground [1] and thermal equilibrium states [1, 2] of local Hamiltonians, or to describe exotic phases of matter [3, 4]. The most prominent examples are matrix product states [5, 6] (MPS), which portray one-dimensional systems, and their higher dimensional generalization, projected entangled-pair states [7] (PEPS). Their simplicity and special properties makes them very practical in numerical computations [8–11], as well as in the characterization and classification of a variety of scenarios and phenomena. This includes, for instance, the characterization of symmetry protected phases in spin [12–14] and fermionic [15] chains, or topological order [4, 16, 17] in two dimensions, lattice gauge theories [18, 19], unitary evolutions [20, 21], one-way quantum computing [7, 22, 23], or quantum tomography [24].

Tensor network states can be defined on arbitrary lattices. They are generated by a set of tensors, $\{A_n\}$, which are assigned to each vertex and are contracted according to the geometry of the lattice. For regular lattices, the generated states are translationally invariant (TI) if all the tensors are the same. A key feature of general TNs is that two different sets of tensors may generate the same tensor network state. This occurs, for instance, when they are related by a (so-called) gauge transformation; that is, when the tensors of one set are related to the other by matrix multiplication of the indices that are contracted, so that those matrices cancel with each other once they are contracted. Let us illustrate this with MPS. There, the tensors A_n have rank three: one of the indices corresponds to the physical index, and the other two to the virtual ones that are contracted in order to generate the state. For a given value of the physical index, i, the tensors are just matrices, A_n^i. Obviously, the tensors B_n, with $B_n^i = X_n A_n^i X_{n+1}^{-1}$, generate the same state as the tensors A_n, where X_n are arbitrary non-singular matrices. One of the fundamental questions in the description of TNs is precisely if this is the only thing that can happen. That is, if two sets of tensors generate the same state, must they be related by a gauge transformation? This question is crucial in many of the applications of tensor networks. For instance, when the answer is affirmative, it gives rise to a canonical form of describing MPS [5, 25, 26]. Or, more importantly, it characterizes the tensors generating states with certain global or local (gauge) symmetries [27, 28]. The reason is very simple: if a state is symmetric it means that an operation leaves it invariant; however, in general, it will change the tensors, so that the resulting ones should be related to the original ones by a gauge transformation. This implies that symmetries in the quantum states can be captured by symmetries in the tensors. This question is also decisive in many other situations dealing with string order [29], topological order [17], renormalization [30], or time evolution [21]. Theorems answering such fundamental questions about the structure of TNs are typically referred to as Fundamental Theorems.

Proving a Fundamental Theorem for the most general TN is impossible: even for two tensors generating translationally invariant 2D PEPS in an $N \times N$ lattice, there cannot exist an algorithm to decide whether they will generate the same state for all N or not [31]. It is therefore necessary to impose restrictions to the TN (both on the geometry of the lattice as well as on the properties of the defining tensors). So far, most of the Fundamental Theorems concern MPS. They have been proven for translationally invariant states [30, 32] as long as the two tensors generate the same state for any size of the lattice. They have also been proven for not necessarily translationally invariant states for a fixed (but large enough) system size for a restricted class of tensors [33]. This class includes injective tensors, that can be inverted by just acting on the physical index, i.e. there exists another tensor, A^{-1}, such that

$$\sum_i A^i_{\alpha,\beta} (A^{-1})^i_{\alpha',\beta'} = \delta_{\alpha,\alpha'} \delta_{\beta,\beta'},$$

as well as normal tensors, that become injective after blocking a few sites. For 2D PEPS such theorems only exist for restricted (but generic) classes of tensors: for normal tensors [33] and semi-injective tensors [34]. These theorems require only a fixed (but large enough) system size. The proof techniques, however, exploit the lattice structure in a fundamental way and thus do not generalize to other geometries.

In this paper we prove the Fundamental Theorem for normal (and thus also injective) PEPS in arbitrary lattices (geometries and dimensions). We obtain that if two sets of such tensors generate the same state, then they must be related by a gauge transformation. This generalizes the previous results as follows. First, we relax the condition of an existence of a sequence of TNs (required in e.g. Ref. 30) so that our results hold for a fixed (but large enough) size. The required system size is smaller than in Ref. 33. Second, the TNs considered here do not need to be translationally invariant, which is important when applying the results to local gauge symmetries. Third, the results hold for any geometry (including, for instance, three dimensions or hyperbolic, as it is used in the constructions of AdS/CFT correspondence

[35, 36]). Additionally, we show that if a TI PEPS defined in a regular lattice is normal although the tensors are different in different sites, then there exists a TI PEPS description with the same bond dimension and where the tensors at every site are the same. Furthermore, the proof presented here uses a new technique: even though it relies on a reduction to the MPS case, this reduction is done in a local way instead of "slicing" a PEPS into an MPS along one dimension.

II. INJECTIVE MPS

In this Section we define non-translational invariant *injective* MPS. We show that two such MPS generate the same state if and only if the generating tensors are related with a gauge transformation (if the MPS contains at least three sites). This extends the previously known results as here we consider (i) a fixed system size and (ii) non-translational invariant MPS with closed boundary conditions.

A non translational invariant MPS on n particles is a state

$$|\Psi\rangle = \sum_i \mathrm{Tr}\{A_1^{i_1} A_2^{i_2} \dots A_n^{i_n}\}|i_1 \dots i_n\rangle,$$

where each i_k runs through a basis of the (finite dimensional) Hilbert space associated to the kth particle and each $A_k^{i_k}$ is a $D_k \times D_{k+1}$ matrix ($D_{n+1} = D_1$). From now on, we will use graphical notation: each tensor is depicted by a dot with lines attached to it. The lines correspond to the different indices of the tensor; joining the lines correspond to contraction of indices. For example, a scalar is represented by a single dot with no lines joinig to it, a vector is represented by a dot with a single line attached to it, a matrix by a dot with two lines attached to it:

$$s = \overset{s}{\bullet}\ , \quad |v\rangle = \overset{v}{\bullet}\!\!-\ , \quad A = \overset{A}{\bullet}\!\!-\!\!-\ ;$$

the scalar product of two vectors, the action of a matrix on a vector and a matrix element can be written as

$$\langle w|v\rangle = \overset{w}{\bullet}\!\!-\!\!-\overset{v}{\bullet}\ , \quad A|v\rangle = \overset{A}{\bullet}\!\!-\!\!-\overset{v}{\bullet}\ , \quad \langle w|A|v\rangle = \overset{w}{\bullet}\!\!-\!\!-\overset{A}{\bullet}\!\!-\!\!-\overset{v}{\bullet}\ .$$

In this notation, the MPS $|\Psi\rangle$ is written as

$$|\Psi\rangle = \boxed{\overset{A_1}{\bullet}\!\!-\!\!-\overset{A_2}{\bullet}\!\!-\!\!-\overset{A_3}{\bullet}\!\!-\!\!-\cdots\!\!-\!\!-\overset{A_n}{\bullet}}\ .$$

An *injective* MPS is an MPS where every tensor – if considered as a map from the virtual level to the physical one – is injective, i.e.

$$\boxed{\begin{array}{c}\bullet\\ A_i\\ \bullet\\ X\end{array}} = 0 \quad \Rightarrow \quad X = 0.$$

This is equivalent to the tensor A_i admitting a one-sided inverse A_i^{-1}:

$$\begin{array}{c}A_i^{-1}\\ \bullet\\ \bullet\\ A_i\end{array} = \sqsupset\!\sqsubset\ .$$

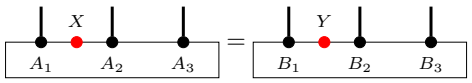
Notice that this immediately shows that the contraction of two injective MPS tensors is again injective; the inverse of the obtained tensor is proportional to the contraction of the inverses of the individual tensors:

$$\begin{array}{c}A_1^{-1}\quad A_2^{-1}\\ \bullet\!\!-\!\!-\!\!-\!\!-\!\!-\!\!-\bullet\\ \bullet\!\!-\!\!-\!\!-\!\!-\!\!-\!\!-\bullet\\ A_1\quad A_2\end{array} = \sqsupset\ \square\ \sqsubset = D \cdot \sqsupset\!\sqsubset\ ,$$

where D is the dimension of the vector space assigned to the index connecting the tensors A_1 and A_2.

In the rest of this Section, we prove the two main lemmas leading to the Fundamental Theorem. We also illustrate how to use them by deriving the Fundamental Theorem for non translational invariant MPS. In the following, we consider two injective tensor networks generating the same state; the defining tensors of the two TNs are labeled by A_i and B_i. The first lemma assigns a special gauge transformation to each edge of one of the tensor networks; the second lemma shows that once these gauges are absorbed into the tensors B_i, the resulting tensors are equal to A_i.

Lemma 1. *Suppose A, B are two injective, non translational invariant MPS on three sites that generate the same state. Then for every edge and for every matrix X there is a matrix Y such that*

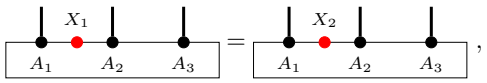


Moreover, X and Y have the same dimension and there is an invertible matrix Z such that $Y = Z^{-1}XZ$. This Z is uniquely defined up to multiplication with a constant.

This Lemma will be used to assign a local gauge transformation to all edges on one of two tensor networks generating the same state. These local gauges will then be incorporated into the defining tensors; doing so will lead to two tensor networks where inserting any matrix X on any bond simultaneously in the two networks gives two new states that are still equal.

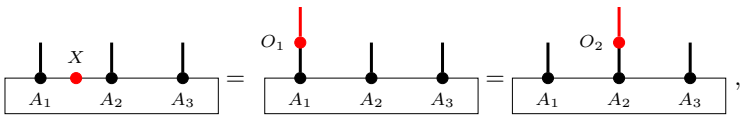
The proof of Lemma 1 is based on the observation that any local operation on the virtual level can be realized by a physical one on either of the neighboring particles; and vice versa, two physical operations on neighboring particles that transform the state the same way correspond to a virtual operation on the bond connecting the two particles. Given two tensor networks generating the same state, this correspondence establishes an isomorphism between the algebra of virtual operations. The basis change realizing this isomorphism is the local gauge relating the two tensors.

Before proceeding to the proof, notice that due to injectivity of the tensors, if

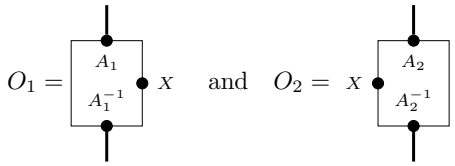


then $X_1 = X_2$.

Proof of Lemma 1. Consider now a deformation of the TN by inserting a matrix X on one of the bonds. This deformation can be realized by physical operations acting on either of the two neighboring particles:



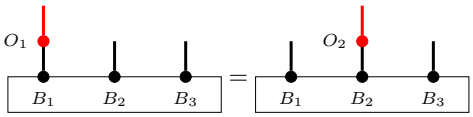
with



(1)

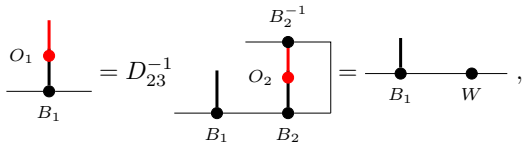
Notice that the mappings $X \mapsto O_1$ and $X \mapsto O_2^T$ are algebra homomorphisms[37]. These mappings do not depend on A_3.

Consider now the converse: two physical operations on neighboring particles that transform the MPS to the same state:



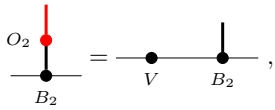
(2)

Inverting B_2 and B_3, we arrive to

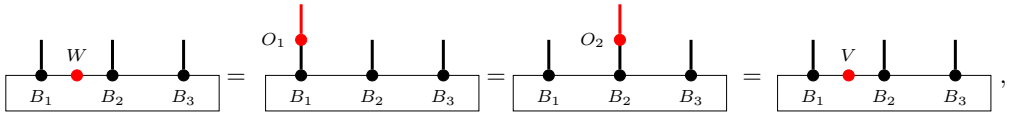


(3)

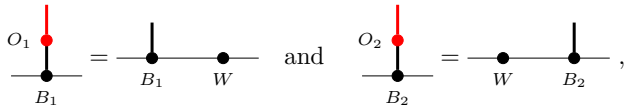
for some matrix W, where D_{23} is the dimension of the vector space on the edge $(2,3)$. Similarly, inverting B_1 and B_3, we arrive to



for some matrix V. Therefore



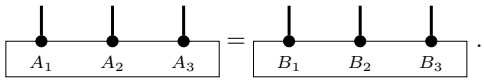
and thus by injectivity, $V = W$. Therefore



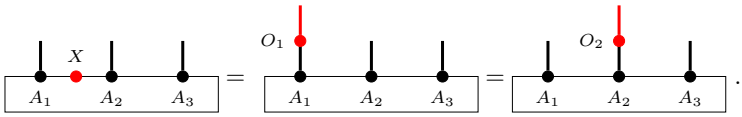
(4)

and the maps $O_1 \mapsto W$ and $O_2^T \mapsto W$ are uniquely defined and are algebra homomorphisms.

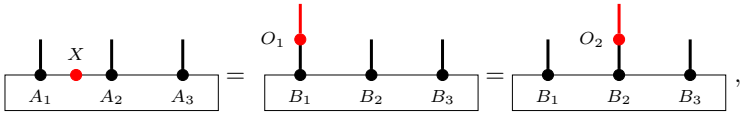
Consider now two three-particle, non translational invariant injective MPS generating the same state:



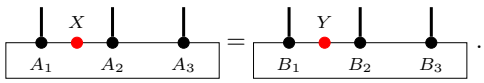
Deform the MPS on the LHS by inserting a matrix X on one of the bonds. By the above arguments, this deformation is equivalent to any of the two physical operations:



As the MPS defined by the A and B tensors is the same state, these physical operators also satisfy

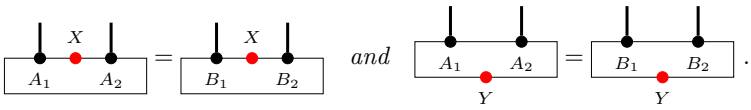


and thus, by Eq. (4), for every X there is a matrix Y such that



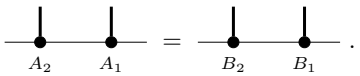
Due to injectivity of the B tensors, the mapping $X \mapsto Y$ is uniquely defined. Due to injectivity of the A tensors, it is an injective map. As the argument is symmetric with respect of the exchange of the A and B tensors, it also has to be surjective and therefore the map $X \mapsto Y$ is a bijection. Moreover, it is clear from the construction that it is an algebra homomorphism, as both $X \mapsto O_1$ and $O_1 \mapsto Y$ are algebra homomorphisms. Therefore the mapping $X \mapsto Y$ is an algebra isomorphism. As X (and Y) can be any matrix on the bond, this means that the bond dimensions on the LHS and the RHS are the same and that $Y = ZXZ^{-1}$ for some invertible Z and this Z is uniquely defined (up to a multiplicative constant). □

Lemma 2. *Let A_1, A_2 and B_1, B_2 be injective MPS tensors. Suppose that for all X and Y*

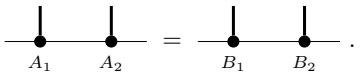


Then $A_1 = \lambda B_1$ and $A_2 = \lambda^{-1} B_2$ for some constant λ.

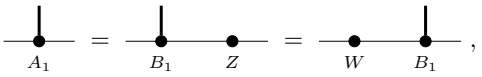
Proof. From the first equation, as X can be any matrix,



Similarly, from the second equation,



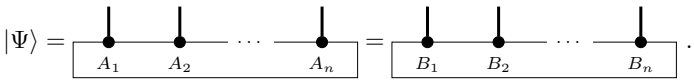
Therefore, applying A_2^{-1} to both equations, we get that



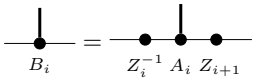
for some matrices Z and W. Applying the inverse of B_1, we conclude that both Z and W are proportional to identity and hence $A_1 = \lambda B_1$. Similarly $A_2 = \mu B_2$ for some other constant μ and $\mu = 1/\lambda$. □

In the following, we show how to use these lemmas for injective MPS to prove the Fundamental Theorem. This is a special case of the next section, and only presented to explain the ideas.

Theorem 1. *Let the tensors A_i and B_i define two injective, non translational invariant MPS on at least three particles. Suppose they generate the same state:*

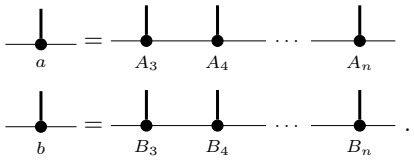


Then there are invertible matrices Z_i ($i = 1, ..., n+1$, $Z_{i+1} = Z_1$) such that

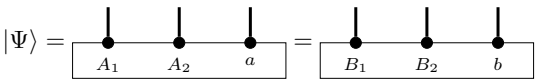


Moreover, the gauges Z_i are unique up to a multiplicative constant.

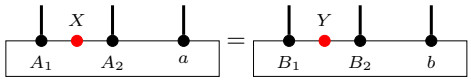
Proof. First let us choose any edge, for example the edge $(1, 2)$. Let us block the tensors $A_3, \dots A_n$ (and $B_3, \dots B_n$) into one tensor:



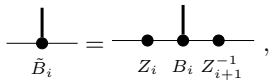
As injectivity is preserved under blocking, both a and b are injective tensors. With this notation, the MPS can be written as a non translational invariant MPS on three sites:



Therefore Lemma 1 can be applied leading to a gauge transform Z_2 on the edge $(1,2)$ that, for all X with $Y = Z_2^{-1} X Z_2$, satisfies

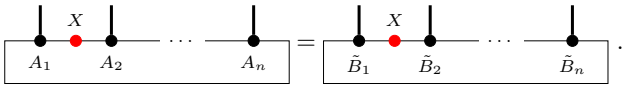


The lemma can be applied to all edges leading to gauge Z_i on the edge $(i-1, i)$. After incorporating these gauges into the tensor B_i:

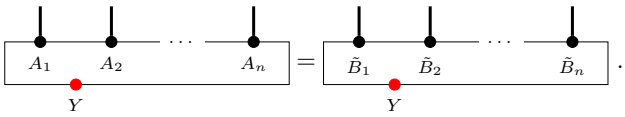


(5)

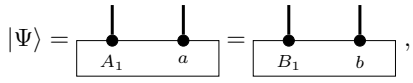
we arrive at two MPS with the property that on every bond for every matrix X



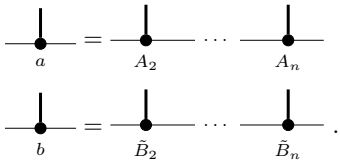
In particular,



Let us now block the MPS into a two partite MPS:

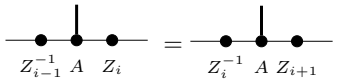


with



After this blocking, the requirements of Lemma 2 are satisfied, therefore $A_1 = \lambda_1 \tilde{B}_1$. Similarly for all i, $A_i = \lambda_i \tilde{B}_i$ and $\prod_i \lambda_i = 1$. Notice that these λ_i can be sequentially absorbed into the gauges Z_i in Eq. (5). □

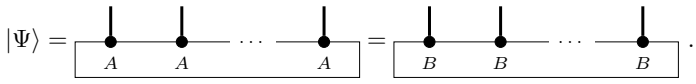
Notice that if the two MPS are translational invariant, i.e. the tensors at each vertex are the same, then the gauges relating them are also translational invariant (up to a constant), as



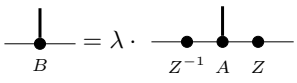
$$\Rightarrow \; Z_i \propto Z_{i+1},$$

which can be seen by inverting the tensor A. We conclude therefore that

Corollary 1. *Let the tensors A and B define two injective, translational invariant MPS on $n \geq 3$ particles. Suppose they generate the same state:*



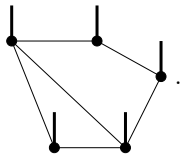
Then there is an invertible matrix Z and a constant $\lambda \in \mathbb{C}$, $\lambda^n = 1$, such that



Moreover, the gauge Z is unique up to a multiplicative constant.

III. INJECTIVE PEPS

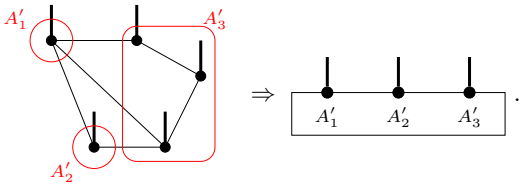
In general, PEPS can be defined on any graph (no double edges are allowed, but there are extra edges attached to every vertex that is associated to a physical particle). The state corresponding to the PEPS is obtained by placing tensors on each vertex and contracting all indices corresponding to the edges of the graph. An example of a tensor network is depicted below:



This definition includes TNs such as MPS, 2D PEPS and higher-dimensional PEPS. It also includes PEPS defined on arbitrary lattices, such as hyperbolic lattices used in the AdS/CFT correspondence[35, 36].

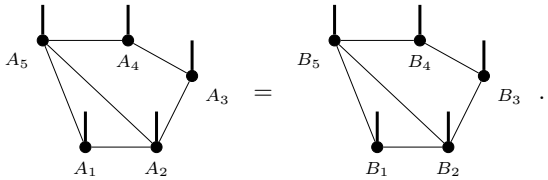
We say that the tensor network is *injective* if all tensors interpreted as maps from the virtual space to the physical one are injective. This is equivalent to the tensor having a one-sided inverse, as in the MPS case. Similar to the MPS case, the contraction of two injective tensors results in an injective tensor.

One can group particles of the PEPS together treating them as one bigger particle. This regrouping can naturally be reflected in PEPS. In particular, we will block tensor networks to a three particle MPS as follows. Choose one edge of the PEPS and group together all vertices except the endpoints of the edge. This regrouped tensor together with the two endpoints of the edge forms a three-partite MPS as illustrated below; notice that the resulting MPS is injective:



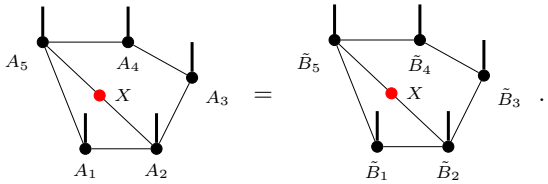
(6)

Consider now two injective PEPS defined on the same graph that generate the same state:



(7)

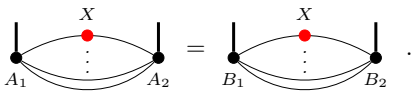
After blocking to MPS as described above, we arrive at two injective MPS generating the same state; hence Lemma 1 can be applied. This establishes a gauge transformation on the edge $(1, 5)$ of the original PEPS. Similar regrouping can be done around every edge; applying then Lemma 1 results in a gauge transformation assigned to every edge. Define now the tensors $\tilde{B}_i$ by absorbing these gauges into the tensors B_i. For the resulting PEPS, we have that for every edge and matrix X



(8)

To conclude that $A_i = \lambda_i \tilde{B}_i$, we will need to use a more general version of Lemma 2:

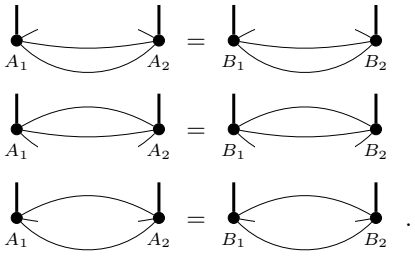
Lemma 3. *Let A_1, A_2 and B_1, B_2 be injective tensors. Suppose for all X on all edges*



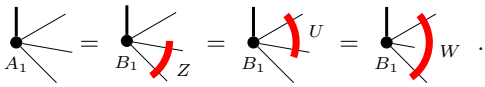
(9)

Then $A_1 = \lambda B_1$ *and* $A_2 = \lambda^{-1} B_2$ *for some constant* λ.

Proof. W.l.o.g. suppose that there are three lines connecting the tensors. Similar to the proof of Lemma 2, if Eq. (9) holds for all X, then



Applying now the inverse of A_2, we conclude that



Inverting B_1 we conclude that the gauges Z, U, W satisfy

$$\sum_i \mathrm{Id} \otimes Z_i^{(1)} \otimes Z_i^{(2)} = \sum_i U_i^{(1)} \otimes U_i^{(2)} \otimes \mathrm{Id} = \sum_i W_i^{(1)} \otimes \mathrm{Id} \otimes W_i^{(2)},$$

where we have written

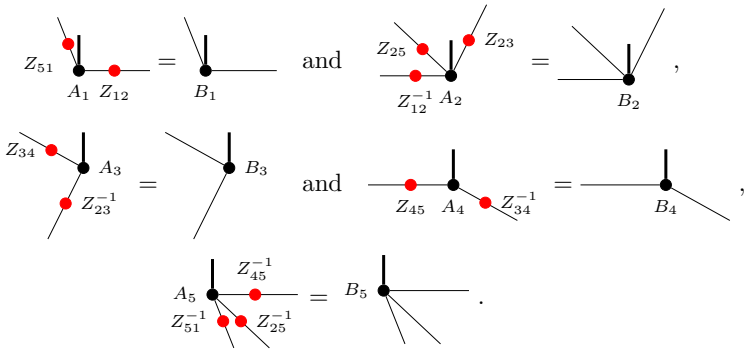
$$Z = \sum_i Z_i^{(1)} \otimes Z_i^{(2)}$$
$$U = \sum_i U_i^{(1)} \otimes U_i^{(2)}$$
$$W = \sum_i W_i^{(1)} \otimes W_i^{(2)} .$$

Therefore all three gauges are proportional to the identity and thus $A_1 = \lambda B_1$. Similarly we get $A_2 = 1/\lambda B_2$. □

Let us now block the PEPS in Eq. (8) into two injective tensors: select one tensor and block all the others into another injective tensor. These PEPS now satisfy the requirements of Lemma 3 and thus for all i, $A_i = \lambda_i \tilde{B}_i$ for some constant λ_i, giving the Fundamental Theorem for general injective PEPS (the constants λ_i can be incorporated into the gauge transformations):

Theorem 2. *Two injective PEPS – defined on a graph that does not contain double edges and self-loops – generate the same state if and only if the generating tensors are related with a local gauge. These gauges are unique up to a multiplicative constant.*

As the defining graph can not contain double edges and self-loops, the theorem is applicable for MPS of size N only if $N \geq 3$, and for 2D PEPS of size $N \times M$ only if both $N \geq 3$ and $M \geq 3$. As an illustration of the theorem, for the two PEPS in Eq. (7) there are matrices $Z_{12}, Z_{23}, Z_{34}, Z_{45}, Z_{51}$ and Z_{25} such that



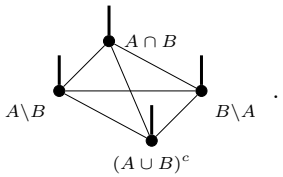
IV. NORMAL PEPS

We call a PEPS *normal*, if blocking tensors in certain regions results in injective tensors. To derive the Fundamental Theorem for this kind of PEPS, we use the same arguments as above after blocking tensors to injective ones. This technique requires that the system is big enough to allow for blocking. This proof technique presented here is not optimal in the required system size; we describe a proof technique giving tighter bounds in Appendix A. For simplicity, we present the proof for a TI normal PEPS on a square lattice, but it can easily be generalized to the non TI case on any geometry.

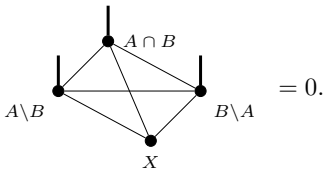
Before proceeding to the proof, we need the following lemma:

Lemma 4. *The union of two injective regions is injective.*

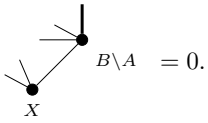
Proof. Let A and B be two injective regions. W.l.o.g. the TN can be blocked as follows (missing edges don't change the proof):



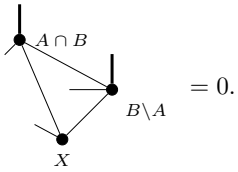
Notice that $A \cup B = (A \backslash B) \cup (A \cap B) \cup (B \backslash A)$. Let X now be a tensor such that



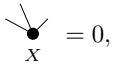
As the region $A = (A \backslash B) \cup (A \cap B)$ is injective,



Plugging back the tensor over the region $A \cap B$,

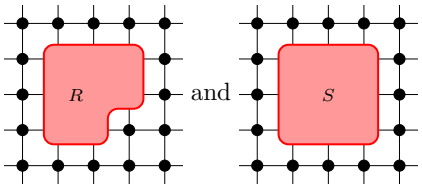


Finally, the region $B = (A \cap B) \cup (B \backslash A)$ is injective, hence inverting the tensor over that region gives

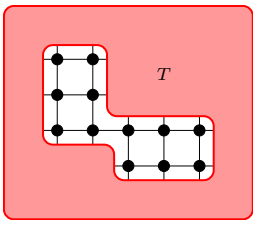


which means that the region $A \cup B$ is injective. □

For example, if in a TI 2D PEPS every 2×3 and 3×2 region is injective, then the following regions:

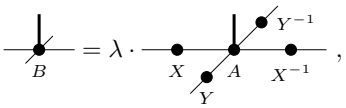


are unions of smaller injective regions, and they are thus injective. Similarly, if the size of the PEPS is at least 5×6, then the region T depicted below is injective:



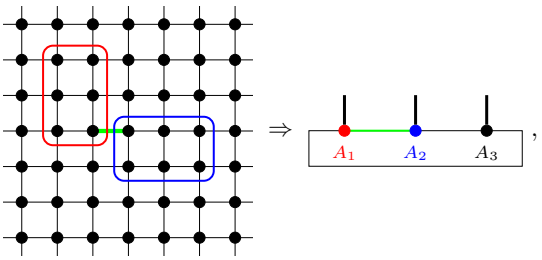
In the following we prove the Fundamental Theorem for a normal TI 2D PEPS. In particular, we prove it in detail for the case where every region of size 2×3 and 3×2 is injective as in the examples above. Then, we generalize the proof for any normal PEPS that is big enough to allow the necessary blockings.

Theorem 3. *Let A and B be two normal 2D PEPS tensors such that every 2×3 and 3×2 region is injective. Suppose they generate the same state on some region $n \times m$ with $n, m \geq 7$. Then A and B are related to each other with a gauge transformation:*



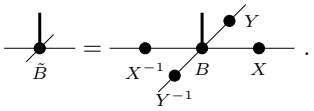
with $\lambda^{n \cdot m} = 1$ and X, Y invertible matrices. X and Y are unique up to a multiplicative constant.

Proof. Let us block the TN into three injective parts around an edge. This can be done with e.g. the following choice of regions:

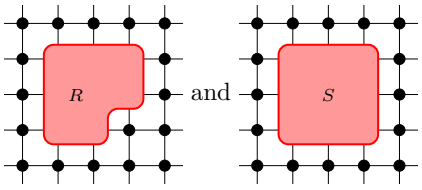


where A_1 corresponds to the red region, A_2 to the blue one and A_3 to the rest. The region A_3 is injective as long as the size of the PEPS is at least 5×7. Therefore a 7×7 PEPS can be blocked to injective three partite MPS around every edge (including the vertical edges that require a PEPS size at least 7×5). Therefore Lemma 1 can be applied giving a gauge transformation on every edge. Due to translation invariance, these gauges are described by the same matrix X (Y) on all horizontal (vertical) edges.

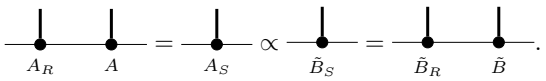
Define now $\tilde{B}$ by incorporating the local gauges into the tensors B, such as in the injective case:



The two PEPS tensors A and $\tilde{B}$ generate the same state. Moreover, inserting a matrix Z on any bond of the first PEPS gives the same state as inserting the same matrix Z on the corresponding bond of the second PEPS. Remember that Lemma 4 implies that both



are injective regions and notice that the two regions differ in a single site. Moreover, if the PEPS is at least 5×5, their complement regions R^c and S^c are also injective. Let us denote the tensor on region R as A_R ($\tilde{B}_R$) and on region S as A_S ($\tilde{B}_S$). Then, by Lemma 3, $A_R \propto \tilde{B}_R$ and $A_S \propto \tilde{B}_S$. This can be represented as



Applying the inverse of $A_R \propto \tilde{B}_R$ on the two ends of the equation, we get that the tensors A and $\tilde{B}$ are proportional. □

The above proof can be repeated for any PEPS as long as it is possible to block into injective regions as required by Lemma 1 and Lemma 3. This leads to the Fundamental Theorem of normal PEPS:

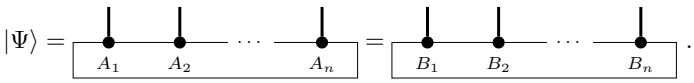
Theorem 4. *Suppose two normal PEPS generating the same state satisfy the following:*

- *they can be blocked into three partite injective MPS around every edge,*
- *and for every site, there are injective regions with their complements also being injective that differ only in the given site.*

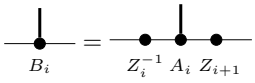
Then the defining tensors are related with a local gauge. Moreover, the gauges are unique up to a multiplicative constant.

Notice that this statement holds for a fixed system size (which is big enough to allow blocking into injective MPS), and translational invariance is not required. In case of a translational invariant system, the gauges are also translational invariant (if the proportionality constants are not absorbed into the gauges). In the following we present some special cases. For non TI MPS, the statement reads as

Corollary 2. *Let $\{A_i\}_{i=1}^n$ and $\{B_i\}_{i=1}^n$ two normal MPS on $n \geq 3L$ sites with the property that blocking any L consecutive sites results in an injective tensor. Suppose they generate the same state:*



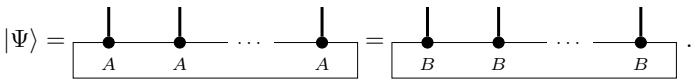
Then there are invertible matrices Z_i (for $i = 1 \ldots n$, $n+1 \equiv 1$) such that for all $i = 1 \ldots n$



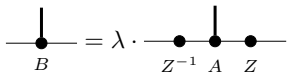
Moreover, the gauges Z_i are unique up to a multiplicative constant.

In Appendix A we strengthen the statement to include system sizes $n \geq 2L + 1$. For TI MPS, the statement reads as

Corollary 3. *Let A and B be two normal TI MPS on $n \geq 3L$ sites with the property that blocking L consecutive sites results in an injective tensor. Suppose they generate the same state:*



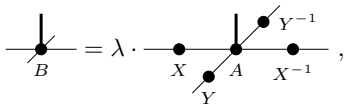
Then there is an invertible matrix Z and a constant λ with $\lambda^n = 1$ such that



Moreover the gauge Z is unique up to a multiplicative constant.

In Appendix A we strengthen the statement to include system sizes $n \geq 2L+1$. For 2D TI PEPS, the statement reads as

Corollary 4. *Let A and B be two normal 2D PEPS tensors such that every $L \times K$ region is injective. Suppose they generate the same state on some region $n \times m$ with $n \geq 3L$ and $m \geq 3K$. Then A and B are related to each other with a gauge:*



with $\lambda^{n \cdot m} = 1$ and X, Y invertible matrices. Moreover these matrices X, Y are unique up to a multiplicative constant.

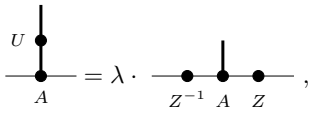
In Appendix A we strengthen the statement to include system sizes $n \geq 2L + 1$ and $m \geq 2K + 1$. Similar statements can be made for the non-TI case as well as for other situations, including PEPS in 3 and higher dimensions, other lattices (e.g. triangular, honeycomb, Kagome), and other geometries (e.g. hyperbolic, as it is used in the AdS/CFT constructions [35, 36]).

Furthermore, the results hold for general tensor networks as well (including tensors that do not have physical index), provided that the TN satisfies the conditions in Theorem 4. However, there is an important class of TN that do not satisfy them, namely the MERA [11], and thus our results do not apply to them.

V. APPLICATIONS

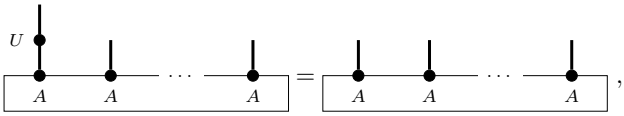
In this Section we show how the above results can be applied in different scenarios. In particular, we consider local (gauge) and global symmetries as well as translation symmetry.

Consider a normal TN on n particles describing a state $|\Psi\rangle$. Suppose $|\Psi\rangle$ admits a global symmetry: $U^{\otimes n}\Psi = \Psi$. Then, if the TN satisfies the conditions in Theorem 4, the symmetry operators acting on the individual tensors is the same as acting with gauge transformations on the virtual level. For example, in TI MPS, this is reflected as:

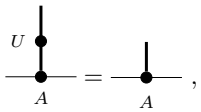


with $\lambda^n = 1$. Similar statements are true in the non TI case (in which case the gauges might be different on every edge) and for any geometry. If the state admits a whole symmetry group, the gauges form a projective representation of that group on every bond.

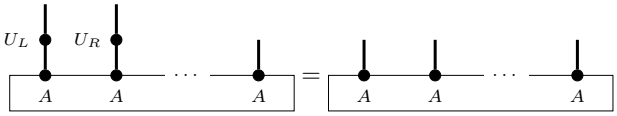
Consider now a local (gauge) symmetry in a normal TN. If the symmetry is strictly one-local, it leaves each tensor invariant. As an illustration, for MPS, if



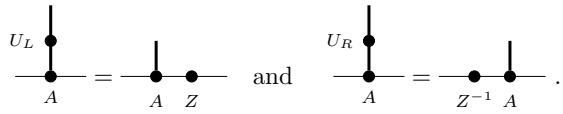
then



as looking at the rest of the tensors, we conclude that all gauges are the identity. For two-local symmetries, if



then

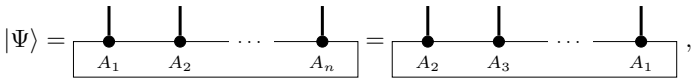


Here, if the state is symmetric under a whole group of unitaries, then the gauge Z forms a linear representation of that group. Similar statements can be obtained for three-local symmetries as well as for any geometry provided that the TN satisfies the conditions in Theorem 4.

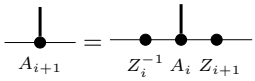
Consider now translation symmetry. We prove that a TI state (defined on a regular lattice) that has a normal PEPS description also has a TI PEPS description with the same bond dimension. This holds, for instance, for injective and normal 2D PEPS and MPS. Below we provide the proof for injective MPS, but the proof can easily be extended to the other cases as well.

Corollary 5. *Let the tensors A_i define an injective MPS such that the resulting state is translational invariant. Then all bond dimensions are the same and the state has a TI MPS description with an injective tensor B that has the same bond dimension.*

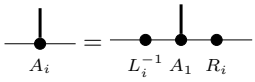
Proof. Translational invariance means



thus, by Theorem 1, there are invertible matrices Z_i such that for all i ($n+1 \equiv 1$)



Therefore all tensors can be expressed with the help of the first tensor (A_1) together with some invertible matrices acting on the virtual dimensions of the tensor:

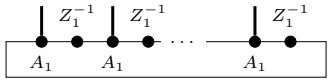


(10)

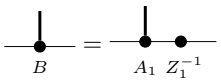
with

$$L_i = Z_1 Z_2 \dots Z_{i-1},$$
$$R_i = Z_2 Z_3 \dots Z_i.$$

As $R_i L_{i+1}^{-1} = Z_1^{-1}$ for all i, substituting A_i as in Eq. (10), the state can be written as



where we have used that $A_{n+1} \equiv A_1$ and thus $R_{n+1} = L_{n+1} = 1$, which means that $R_n = Z_2 \dots Z_n = Z_1^{-1}$. This means that the state admits a TI MPS description with the tensor



□

The corresponding statement for injective 2D PEPS is

Corollary 6. *Let the tensors $A_{(i,j)}$ define an injective 2D PEPS such that the resulting state is translational invariant. Then all vertical (resp. all horizontal) bond dimensions are the same and the state has a TI 2D PEPS description with an injective tensor B that has the same bond dimension.*

VI. CONCLUSION

In this paper we have shown the 'Fundamental Theorem' for injective and normal PEPS: two such tensor networks generate the same state if and only if the defining tensors are related with a local gauge. Moreover, the gauges relating the two set of tensors are uniquely defined up to a multiplicative constant. This result holds for a fixed (but large enough) system size. It is valid for any geometry, TI and non-TI setting, including 1D (MPS), 2D PEPS, higher dimensional PEPS, and other lattice geometries such as the honeycomb lattice, the Kagome lattice and the hyperbolic lattice used in the AdS/CFT correspondence. However, it does not include some important classes of TN like MERA, since they do not meet the conditions of Theorem 4.

VII. ACKNOWLEDGEMENTS

We thank Barbara Kraus, David Sauerwein, Erez Zohar and Ilya Kull for inspiring conversations.

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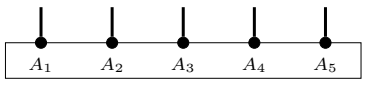
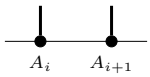
Appendix A: Normal MPS: alternative proof

In Section IV we have shown that two normal TNs generate the same state if and only if the generating tensors are related with a gauge transformation. In the proof, we have blocked tensors to injective tensors. This proof is not optimal in the system size. For example, consider an MPS on five sites

$|\Psi\rangle =$ 

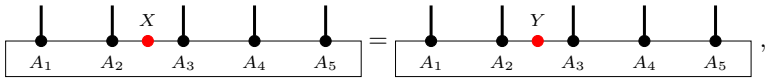
,

where the blocking of any two consecutive tensors:



is injective. The proof in Section IV does not work for this case as this MPS cannot be blocked to a three-partite injective MPS (as it is too short). Here we prove a more size-efficient variant of Lemma 1 for this situation.

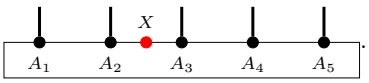
Lemma 4 implies that any region of at least size two is also injective. Now, similar to the injective case, for every edge and every matrix X and Y, if



,

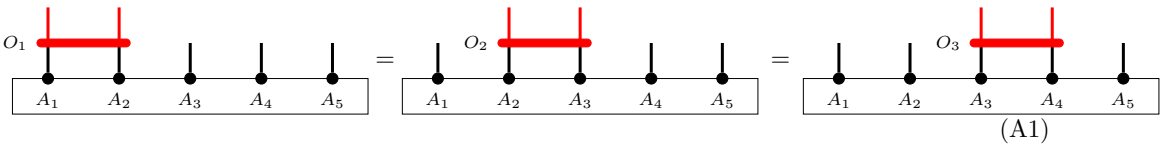
then $X = Y$.

Consider now any virtual operation X on a given edge:

$|\Psi'\rangle =$ 

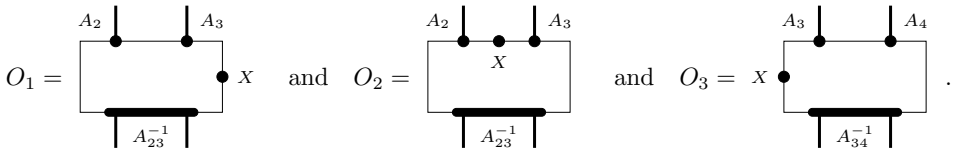
.

This operation can also be realized by three different two-local physical operators:

$|\Psi'\rangle =$ 

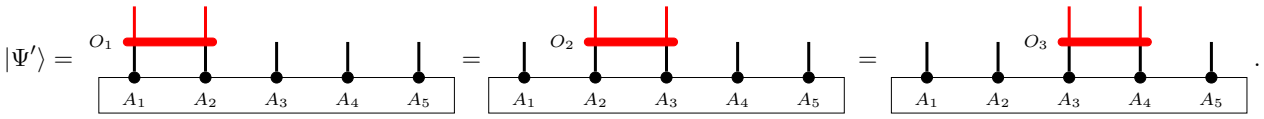
, (A1)

with

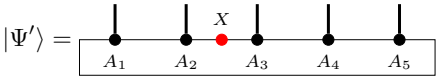


Notice that both $X \mapsto O_1$ and $X \mapsto O_3^T$ are algebra homomorphisms, but the map $X \mapsto O_2$ not necessarily. Conversely:

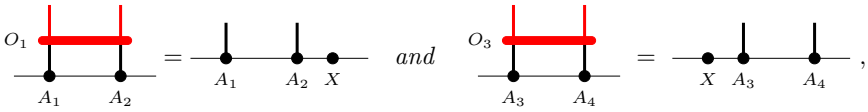
Lemma 5. *Suppose that the state $|\Psi'\rangle$ can be written as*



Then there is a virtual operation X on the bond $(2,3)$ such that

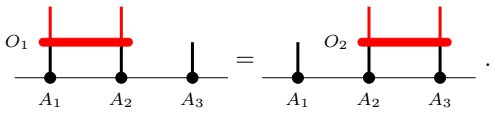


moreover,



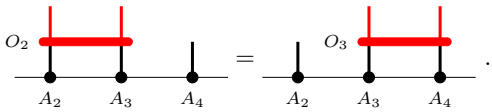
and the maps $O_1 \mapsto X$ and $O_3^T \mapsto X$ are uniquely defined and are algebra-homomorphisms.

Proof. Invert the injective tensor on the region 45. We get



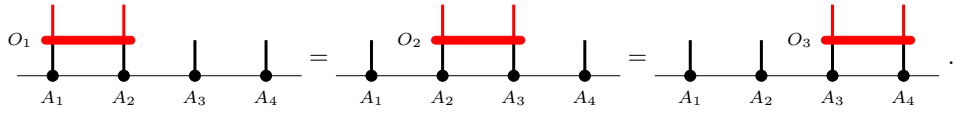
(A2)

Similarly, inverting the tensor on the region 51, we get

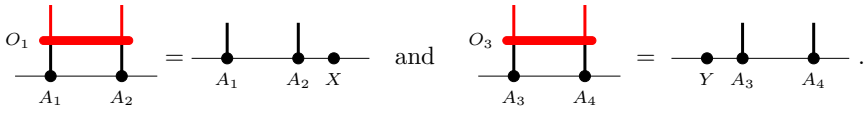


(A3)

Therefore, plugging A_4 on the right side in Eq. (A2) and A_1 on the left side in Eq. (A3), we get



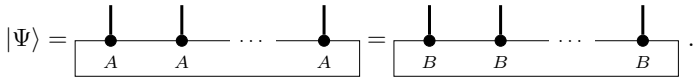
Comparing the two ends of the equation, similar to Eq. (3), we get that



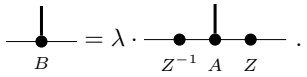
Finally $X = Y$ by comparing the states they generate. These relations define X uniquely and by composition, the maps $O_1 \mapsto X$ and $O_3 \mapsto X^T$ are algebra homomorphisms. □

Notice that similar to the injective case, this leads to

Corollary 7. *Let A and B be two normal TI MPS on $n \geq 2L+1$ sites with the property that blocking L consecutive sites results in an injective tensor. Suppose they generate the same state:*



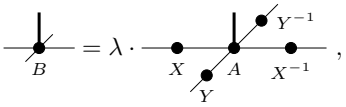
Then there is an invertible matrix Z and a constant λ with $\lambda^n = 1$ such that



Moreover the gauge Z is unique up to a multiplicative constant.

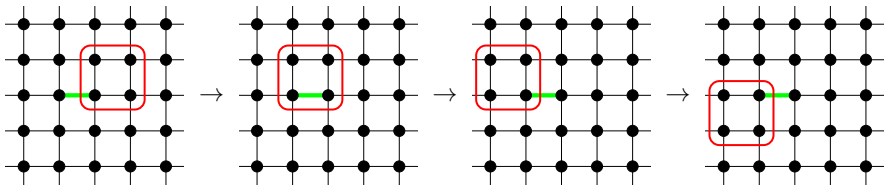
The arguments in Lemma 5 can be applied for 2D PEPS as well. In the TI setting, this leads to

Corollary 8. *Let A and B be two normal 2D PEPS tensors such that every $L \times K$ region is injective. Suppose they generate the same state on some region $n \times m$ with $n \geq 2L+1$ and $m \geq 2K+1$. Then A and B are related to each other with a gauge:*

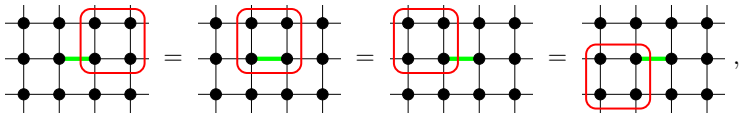


with $\lambda^{n \cdot m} = 1$ and X, Y invertible matrices. Moreover these matrices X, Y are unique up to a multiplicative constant.

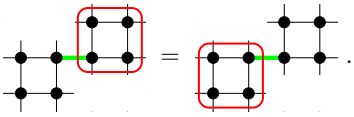
Sketch of proof. We only need to prove a statement similar to Lemma 5. For that, notice that a virtual operation on a given bond can be interpreted as a physical operation on any of the following four regions (in the case of $K = L = 2$):



We need to prove that conversely, any four physical operators on the above regions that transforms the PEPS into the same state means that the transformation can equally be done with a virtual operation on the highlighted edge. The system size required to compare any two consecutive regions is only 5×5 (and in general, $(2L+1) \times (2K+1)$). Therefore, similar to Lemma 5,



with open boundaries. Compare now the first and the last expression in the above equation. One can add two-two tensors in the upper left and lower right corner and invert the resulting regions, leading to



This results in the desired virtual operation on the highlighted edge. The rest of the proof is the same as the proof of Theorem 3. □

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3.6 Computational complexity of PEPS zero testing

In this Chapter we include the following paper:

- G. Scarpa et al. "Computational complexity of PEPS zero testing". In: *ArXiv e-prints* (Feb. 22, 2018). arXiv: 1802.08214

In the previous Section we proved a fundamental theorem for normal tensors: provided locally checkable conditions under which such set of tensors generate the same state. However, in some cases fundamental theorems are used under different conditions. For example, in Section 3.3 the fundamental theorem used to classify MPO representations of groups requires only one of the two MPS tensors to be normal. In fact, the typical use of fundamental theorems require this kind of asymmetric conditions. For example, both the characterization of renormalization fixed points of MPDOs [72] and the classification of MPUs with and without symmetries [72, 73] use this condition. It is natural to ask therefore how the conditions in Section 3.5 can be relaxed. In this Section we show that such a weakening of the conditions is not possible for PEPS: given two TI PEPS tensors such that only one of them is normal, there cannot be a locally checkable condition deciding whether they generate the same state.

In this project, we construct examples for PEPS for which it is hard to check whether they generate the zero state. For finite system size with open boundary condition verifying that the PEPS generates the zero state is NP-hard, whereas the same question for periodic boundary conditions and all system sizes is an undecidable problem. More precisely, it is impossible to find an algorithm that halts for all input PEPS tensors whose task is to decide whether the given input generates zero for every system size. The main idea behind the proof is to encode the tiling problem (and thus the halting problem of Turing machines) into the question whether a given PEPS is zero.

This statement has far-reaching consequences for the fundamental theorems. For example, given two general tensors, there can not be an algorithm that always decides whether they generate the same state. Therefore one has to restrict the input of the algorithm to certain classes of tensors such as normal tensors. Note that restricting only one of the two inputs is not enough. Since the zero state is generated by a normal tensor (the zero tensor), comparing an arbitrary tensor with zero is a special case of comparing an arbitrary tensor with a normal one. This means that a classification of PEPS operator representation of groups (the direct generalization of MPO representations) is a much harder task then its one-dimensional counterpart.

The importance of this project is therefore that it provides an understanding of what kind of fundamental theorems can be expected to hold in two dimensions. As the compared tensors have to be restricted to certain classes, one has to understand which classes of tensors behave well. We expect that G-injective and MPO-injective tensors describing topological models are classes for which there is a fundamental theorem.

Computational complexity of PEPS zero testing

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(Dated: February 23, 2018)

Projected entangled pair states aim at describing lattice systems in two spatial dimensions that obey an area law. They are specified by associating a tensor with each site, and they are generated by patching these tensors. We consider the problem of determining whether the state resulting from this patching is null, and prove it to be NP-hard; the PEPS used to prove this claim have a boundary and are homogeneous in their bulk. A variation of this problem is next shown to be undecidable. These results have various implications: they question the possibility of a 'fundamental theorem' for PEPS; there are PEPS for which the presence of a symmetry is undecidable; there exist parent hamiltonians of PEPS for which the existence of a gap above the ground state is undecidable. En passant, we identify a family of classical Hamiltonians, with nearest neighbour interactions, and translationally invariant in their bulk, for which the commuting 2-local Hamiltonian problem is NP-complete.

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

However, a formidable difficulty arises when one attempts to actually use these states. Generically, evaluating mean values of physical observables turns out to be a #P-hard problem, and a black box that prepares PEPS would allow to solve PP problems [6]. In this landscape, it is legitimate to look at the complexity of a simpler question: what is the complexity of deciding whether a given tensor network state is naught? For *general* tensor network states, this problem has been proven to be NP-hard [7].

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

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

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

where each $A_k(s)$ is a matrix. Namely, all $A_k(s)$ have a fixed size $D\times D$ for $k=2\dots n-1$, while the matrices $A_1(s)$ have dimensions $1\times D$, and the matrices $A_n(s)$ have dimensions $D\times 1$ (open boundary conditions assumed). It has been proven that the ground states of one-dimensional gapped quantum systems are well represented by MPS whose bond dimension D does not depend on n [9–11]. One can observe that the number of parameters necessary to specify an MPS, ndD^2 complex numbers, only grows linearly with n, whereas the dimension of the full Hilbert space where it lives grows exponentially with n. The higher D, the more entanglement can be represented. MPS allow for a diagrammatic description specified by two rules: (i) a tensor is represented by a vertex with a number of legs sticking out equal to the number of indices of the tensor, (ii) summation over repeated indices amounts to glueing legs. With these two rules, Eq.(1) is equivalent to Fig. 1.

A PEPS is a two-dimensional generalisation of Fig. 1.

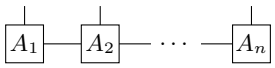

Figure 1. Diagrammatic representation of an MPS.

Fig.2 is an example of a 4×5 PEPS (open boundary conditions assumed). More formally, a PEPS is constructed through association of a $(4+1)$-index tensor $A^{udlr}_{(k,l)}(s)$ with each lattice site (k,l). The analogue of the ansatz (1) on an $m \times n$ square lattice is:

$$\sum_{s_{11}\dots s_{mn}=1}^{d} \mathcal{C}[A_{11}(s_{11}),\dots,A_{mn}(s_{mn})]|s_{11}\dots s_{mn}\rangle, \quad (2)$$

where $\mathcal{C}$ denotes the contraction (*i.e.* summation) over the repeated 'up','down','left','right' virtual indices.

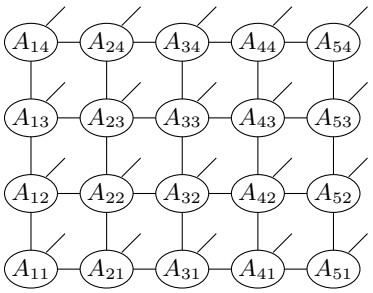

Figure 2. Diagrammatic representation of a 4×5 PEPS. The diagonal legs represent physical degrees of freedom, whereas horizontal and vertical legs represent virtual degrees of freedom.

Given a square lattice with an edge and no hole, and a PEPS tensor associated with each of its sites, does the operation of glueing the tensor legs along the edges of the lattice result in a non-zero state? We address this question through a relation with tiling problems. Given a finite *set of colours* Γ, a *tile set* T is any set of four-letter words $\mathbf{w} = (w_u, w_d, w_l, w_r) \in \Gamma^4$. Considering a square lattice Λ, a boundary condition is the specification of a colour with each link of the boundary, and a tiling is any assignment of a colour with each link of the lattice. Given a boundary condition, a tiling is *valid* if the 4-tuple of colours around each plaquette belongs to the tile set, and if the boundary condition is respected. The bounded tiling (BT) problem has an input defined by a set of colours, a boundary condition, a tile set, and consists in deciding whether a valid tiling exists.

Theorem 1. *Bounded tiling is NP-complete [12].*

The proof of this important theorem is reviewed in Appendix A; it relies on the encoding of the evolution of a universal Turing machine into a BT problem.

BT admits a 'local' formulation in terms of a classical nearest-neighbour *Hamiltonian*. We consider a square lattice Λ where four colour degrees of freedom (u,d,l,r) live at the centre of each plaquette. The energy operator is

$$H^{\mathsf{BT}} = \sum_{\langle p,p'\rangle} h^{\mathsf{T}}_{p,p'} + \sum_{p\in\partial\Lambda} h^{\mathsf{T},\partial}_{p}. \quad (3)$$

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

$$h^{\mathsf{T}}_{p,p'} = \mathbf{1}^{\otimes 8}_{\Gamma} - \sum_{\mathbf{w},\mathbf{w}'\in T} \delta(w_l, w'_r)\ |\mathbf{w},\mathbf{w}'\rangle\langle\mathbf{w},\mathbf{w}'|.$$

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

$$h^{\mathsf{T},\partial}_{p} = \mathbf{1}^{\otimes 4}_{\Gamma} - \sum_{\mathbf{w}\in T} \delta(w_u, \gamma_p)\ |\mathbf{w}\rangle\langle\mathbf{w}|.$$

It is obvious that $H^{\mathsf{BT}} \geq 0$ and that the ground state energy of H_{BT} is zero if and only if the associated BT problem admits a solution. This observation allows to relate the BT problem with the k-local Hamiltonian problem. In the latter, the input is a Hamiltonian H and two real parameters α, β. The Hamiltonian acts on n qudits and is a sum of k-body terms; α and β satisfy $\alpha - \beta \geq 1/\mathsf{poly}(n)$. The task is to decide whether the ground state energy of H is at most α or at least β. What makes this problem interesting is its computational power. For instance, quantum 2-local Hamiltonian is QMA-complete [14]. Versions of the problem where all the terms appearing in the Hamiltonian commute (CLH) are computationally interesting too. For instance, there is a variant of a problem, involving qubit plaquette interactions which is in NP [16]. For more results on the CLH problem, see [15]. The Hamiltonian (3) associated with BT allows to make an observation along these lines. We get the following result.

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

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

We now turn back to the main issue of this paper, and consider a PEPS $|\Phi_{\mathsf{BT}}\rangle$ defined as follows. In the bulk,

$$A^{(\mathbf{w})}_{\mathsf{T}}(\mathbf{s}) = \sum_{\mathbf{w}'\in T} \delta(\mathbf{w},\mathbf{w}')\delta(\mathbf{w},\mathbf{s}). \quad (4)$$

On a top edge plaquette with colour set to some value γ,

$$A^{(\gamma,w_d,w_l,w_r)}_{\mathsf{T},\mathsf{top}}(\mathbf{s}) = \sum_{\mathbf{w}'\in T} \delta(\{\gamma,w_d,w_l,w_r\},\mathbf{w}')\delta(\mathbf{w}',\mathbf{s}).$$

The tensors are given by similar expressions for the three other edges and for the four corners. Since tensors on neighbouring sites are patched by identifying left/right or up/down virtual indices, we see that $|\Phi_{\mathsf{BT}}\rangle$ is the sum of all classical configurations of colours that automatically satisfy the constraint that the colours of adjacent plaquettes should match, and comply the boundary condition. Therefore, $|\Phi_{\mathsf{BT}}\rangle \neq 0$ if and only if BT admits a solution; actually $|\Phi_{\mathsf{BT}}\rangle$, when non-zero is a ground state of H_{BT}. This observation, combined with Theorem 1, proves the following:

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

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

It is well known that there is no algorithm, however inefficient, that receives any finite tile set T as input, and correctly decides whether there exists a periodic tiling of the plane with T [18]: the problem is algorithmically undecidable (see Appendix B). As in the above case where there is a boundary, we can associate a PEPS with the problem of tiling the plane periodically or, equivalently, an $\ell_x \times \ell_y$ torus. This state is obtained by patching the tensor (4) $\ell_x \times \ell_y$ times, with periodic identification. This PEPS is non-zero if and only if a tiling of the plane with periods (ℓ_x, ℓ_y) exists. We conclude the following.

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

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

In the rest of the paper, we discuss three implications of our findings. A first implication is concerned with symmetries. Let $|\Phi_{\mathsf{T}}\rangle$ denote the state resulting from patching the tensor (4) around a torus, and consider $|\Phi\rangle = |\Phi_S\rangle + |\Phi_{\mathsf{T}}\rangle$, where $|\Phi_S\rangle$ denotes a state invariant under some symmetry that $|\Phi_{\mathsf{T}}\rangle$ lacks. $|\Phi\rangle$ admits a PEPS description where the local tensor is the direct sum of the local tensors for $|\Phi_S\rangle$ and $|\Phi_{\mathsf{T}}\rangle$. We see that we can claim that $|\Phi\rangle$ has the symmetry iff we can determine whether $|\Phi_{\mathsf{T}}\rangle = 0$. Therefore, there cannot be a necessary and sufficient *algorithmically decidable* condition for a PEPS to have a symmetry; this situation sharply contrasts with the one-dimensional case [22].

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

$$\mathcal{T}(f(A_k)) = f(A'_k).$$

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

Our third implication is concerned with spectral properties. The undecidability of the spectral gap for short-range Hamiltonians has been established in [8]. We now show that even if we restrict to Hamiltonians that are parent Hamiltonians of a PEPS, undecidability still holds, at least in the case of a finite but unbounded local physical dimension. For that purpose, let us recall a standard procedure to associate a nearest neighbour parent hamiltonian with a PEPS described by a tensor A [21]. With any region R of the lattice, we associate a linear map

$$\chi(A,R) : \left(\mathbb{C}^D\right)^{\otimes|\partial R|} \to \left(\mathbb{C}^d\right)^{\otimes|R|} : |C\rangle \to \sum_{i_R} \mathcal{C}[A_{i_R}C]|i_R\rangle.$$

A parent Hamiltonian is any nearest neighbour Hamiltonian $H = \sum_{\langle p,p'\rangle} h_{p,p'}$, such that $h_{p,p'} \geq 0$, and such that

$$\text{Ker } h_{p,p'} = \text{Im } \chi(A_{\mathsf{T}}, p \cup p'). \tag{5}$$

Such a construction for the tensor (4) yields a parent Hamiltonian $H'_T = \sum_{\langle p,p'\rangle} h'_{p,p'}$ such that $h'_{p,p'} \geq h^{\mathsf{T}}_{p,p'}$, for any pair of neighbouring plaquettes p, p'. This relation follows from the fact that both $h'_{p,p'}$ and $h^{\mathsf{T}}_{p,p'}$ have 0 and 1 as unique eigenvalues, and from the inclusion $\text{Im } \chi(A_{\mathsf{T}}, p \cup p') \subseteq \ker h^{\mathsf{T}}_{p,p'}$. To derive an undecidability result, we will consider an infinite square lattice where each particle lives in a local Hilbert space of the form

$$\mathcal{H} = \mathcal{H}_1 \oplus \left(\mathcal{H}_2 \otimes \mathcal{H}_\Gamma\right).$$

For this system, we will be interested in the state

$$|\Psi\rangle = |\Psi_G\rangle + |\Psi_Z\rangle \otimes |\Phi_{\mathsf{T}}\rangle,$$

where $|\Psi_G\rangle$ is a PEPS living in $\mathcal{H}_1^{\otimes n}$, and where $|\Psi_Z\rangle$ is a PEPS living in $\mathcal{H}_2^{\otimes n}$. $|\Psi\rangle$ is clearly a PEPS: its local tensor is given by

$$A = A_G \oplus (A_Z \otimes A_{\mathsf{T}}). \tag{6}$$

One easily proves the identity

$$\text{Im } \chi(A, R) = \text{Im } \chi(A_G, R) \oplus \{\text{Im } \chi(A_Z, R) \otimes \text{Im } \chi(A_{\mathsf{BT}}, R)\}$$

for any region R. To make our point, it will be enough that $\mathcal{H}_1$ be one-dimensional, and its (unique) basis state will be denoted by $|0\rangle$. We will also choose Ψ_Z to be such that its parent Hamiltonian is gapless and has Ψ_Z as unique ground state, *e.g.* the Ising PEPS discussed in [5] at the critical point. Mimicking the construction of [8], we look at a Hamiltonian described by the two-body interaction

$$h_{pp'} = |0\rangle\langle 0|_p \otimes \mathbf{1}_{p'}^{ZT} + \mathbf{1}_p^{ZT} \otimes |0\rangle\langle 0|_{p'}$$

$$+ h_{pp'}^{Z} \otimes \mathbf{1}_{pp'}^{T} + \mathbf{1}_{pp'}^{Z} \otimes h_{pp'}'. \tag{7}$$

$h_{pp'}$ is evidently a semi-definite positive operator. In order to prove that $H = \sum_{\langle p,p'\rangle} h_{pp'}$ is a parent Hamiltonian for (6), we prove that $\ker h_{p,p'} \subseteq \text{Im } \chi(A, p \cup p')$. Consider then some state $|\phi\rangle \in \ker h_{p,p'}$. The first two penalty terms imply that $|\phi\rangle = |00\rangle_{pp'} + |\phi_{ZT}\rangle_{pp'}$, where $|\phi_{ZT}\rangle_{pp'} \in (\mathcal{H}_2 \otimes \mathcal{H}_\Gamma)^{\otimes 2}$. Clearly, $|00\rangle_{pp'} \in \text{Im } \chi(A_G, p \cup p')$ and $|00\rangle_{pp'} \in \ker h_{p,p'}$. Therefore $|\phi\rangle \in \ker h_{p,p'}$ if and only if $|\phi_{ZT}\rangle \in \ker h_{p,p'}$. This latter condition can only be met if $h_{pp'}^{Z} \otimes \mathbf{1}_{pp'}^{T} |\phi_{ZT}\rangle = 0$, and if $\mathbf{1}_{pp'}^{Z} \otimes h_{pp'}^{\prime T} |\phi_{ZT}\rangle = 0$. That is,

$$\phi_{ZT} \in \{\text{Im } \chi(A_Z, p \cup p') \otimes \mathcal{H}_{pp'}^{T}\} \cap \{\mathcal{H}_{pp'}^{Z} \otimes \text{Im } \chi(A_T, p \cup p')\}$$

$$= \text{Im } \chi(A_Z, p \cup p') \otimes \text{Im } \chi(A_T, p \cup p').$$

Thus, $\phi \in \text{Im } \chi(A, p \cup p')$. The inclusion $\ker h_{p,p'} \supseteq \text{Im } \chi(A, p \cup p')$ is proven likewise. Using the property that $h_{pp'}' \geq h_{pp'}^{\mathsf{T}}$ allows to recycle the argument exposed in Theorem 7 of Section 5.1 of [8], and prove:

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

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

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

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Appendix A: Turing machines and bounded tilings

In this Appendix we define the Bounded Tiling (BT) problem and show its NP-completeness. We start with the necessary definitions [3].

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

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

The set Σ includes a special blank symbol #, and the set K includes the initial state q_0 and the final accepting state q_F.

The machine is *initialised* by writing an input (a non-blank sequence of symbols from Σ) on the tape, positioning the head to the leftmost symbol of the input, and preparing it in the state q_0. A *computation*, then, is a sequence of actions each governed by some quintuple of the program as follows: If the register contains the state q and the head reads on the tape the symbol s, a quintuple of the form $(q, s, ...)$ is selected. On instruction (q, s, q', s', M) the register is updated to q', the symbol s' is written on the tape and the head is moved in the direction given by M. The Turing machine *halts* when no suitable instruction exists to continue, and it *accepts* the input when it halts with the state q_F written in the register. (One can always modify a machine so that halting and accepting coincide, *i.e.,* it halts if and only if it accepts.)

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

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

$$\ldots, \#, \#, s_1, s_2, s_3, q, s_4, s_5, \#, \#, \ldots,$$

which is a way to represent a machine with the head in state q pointing at the fourth cell, and reading s_4. As another example, after instruction (q, s_4, q', s'_4, L) the ID is

$$\ldots, \#, \#, s_1, s_2, q', s_3, s'_4, s_5, \#, \#, \ldots$$

One can represent a t-step computation with a sequence of IDs $T_0, T_1, ..., T_t$ so that each step T_i, T_{i+1} is consistent with some instruction from the program. Then, a machine accepts an input w if and only if there is a sequence of IDs where $T_0 = \ldots, \#, q_0, w, \#, \ldots$ and $T_t = \ldots, \#, q_F, w, \#, \ldots$ We then say that there exists an *accepting* computation for w with this TM.

Turing showed in his seminal paper [1] that there are *universal* Turing Machines (UTMs): machines that can simulate with polynomial overhead any other machine by accepting its description as part of the input. In other words, for every machine T (described by a bitstring t) on input x, the universal TM U satisfies

$$U(t, x) = T(x),$$

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

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

Languages can be arranged in complexity classes, according to the resources needed by a TM to accept them. Two fundamental classes are P and NP. A language L is in P (resp. NP) if there exists a deterministic (resp.

non-deterministic) TM accepting L with computations that take a number of steps polynomial in the length of w (polynomial-time computations). P is obviously contained in NP.

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

$$q_F, \#, \#, \dots$$

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

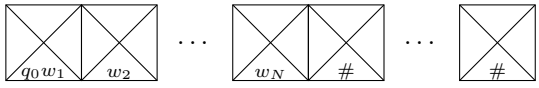

Figure 3. The first row of tiles, corresponding to the initial ID.

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

Conversely, one can show that BT is in NP. Indeed, the notion of certificates for languages in NP (see [3, Section 2.1]), easily provides a deterministic Turing Machine verifying BT in polynomial time given a certificate. (An example for BT is a solution itself.) From this, a standard construction gives a non-deterministic TM that accepts the input iff a certificate (and therefore a solution) exists.

In conclusion, BT is NP-complete.

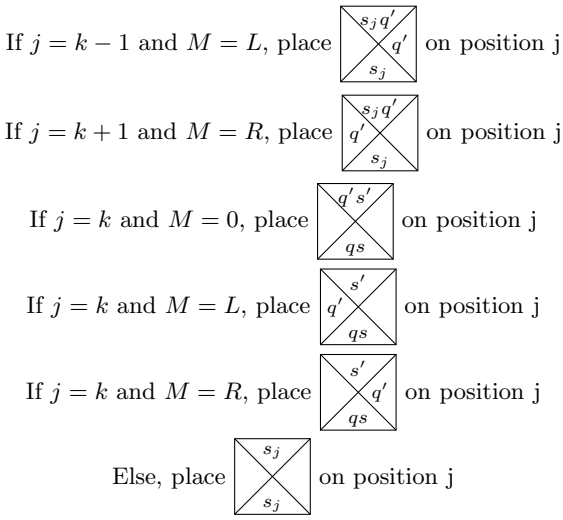

Figure 4. The set of allowed tiles, to which we need to add the empty tile and the tiles with just the top or bottom color corresponding to a symbol from Σ or $\Sigma \times K$.

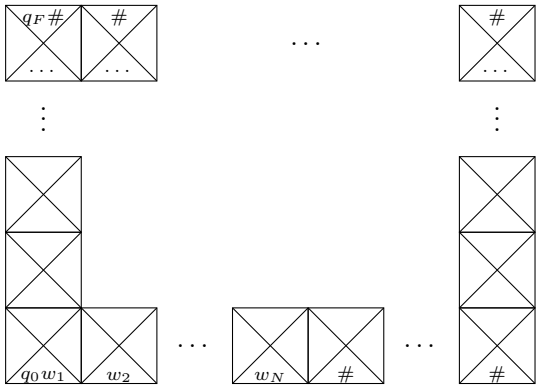

Figure 5. The boundary conditions for the reduction. On the bottom, there is the initial ID, and on the top we enforce the accepting ID.

Appendix B: Undecidability

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

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

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

one that provides the correct answer for every instance: the problem is decidable.

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

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

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3.7 Entanglement of MPS

In this Chapter we include the following paper:

- David Sauerwein, Andras Molnar, J. Ignacio Cirac, and Barbara Kraus. "Matrix Product States: Entanglement, symmetries, and state transformations". In: *arXiv e-prints*, arXiv:1901.07448 (Jan. 2019), arXiv:1901.07448. arXiv: 1901.07448

Entanglement serves as an essential resource for many striking applications in quantum information theory such as in quantum computation [76], in quantum error correction [77], or in quantum secret sharing [78, 79]. We have seen in the previous Chapters that it also plays an essential role in the understanding of many-body systems. Despite its fundamental importance, multipartite entanglement is not yet well understood.

Entanglement is a resource theory where the free operations are are those that can be realized by local operations and classical communication (LOCC). These operations can be realized by many parties manipulating a shared quantum state and they do not increase the entanglement of the state. If the state $|\Phi\rangle$ can be transformed to $|\Psi\rangle$ with LOCC operations, $|\Phi\rangle \xrightarrow{LOCC} |\Psi\rangle$, then $|\Phi\rangle$ is at least as entangled as $|\Phi\rangle$. Therefore the LOCC operations induce a physically relevant partial ordering on the set of quantum states, and the goal of entanglement theory is to unravel this partial ordering. Achieving this goal is very hard to carry out in general, especially because LOCC operations do not admit a well-behaved characterization. One way around this is to investigate, instead, a larger set of transformations that are easier to characterize.

One such class is the set of stochastic LOCC (SLOCC) transformations. In SLOCC transformations, we allow for the protocol to succeed with probability smaller than one. The state $|\Phi\rangle$ can be transformed to another state $|\Psi\rangle$ via SLOCC transformations if one can write $|\Psi\rangle = O_1 \otimes \cdots \otimes O_n |\Phi\rangle$ for some local (maybe singular) operators $O_1, \ldots, O_n$. In this case, we write $|\Phi\rangle \xrightarrow{SLOCC} |\Psi\rangle$. The two states are SLOCC equivalent, $|\Phi\rangle \xleftrightarrow{SLOCC} |\Psi\rangle$, if this relation holds with invertible operators $O_1, \ldots, O_n$. As LOCC operations are a subclass of SLOCC, a classification of SLOCC equivalence classes (and one-way transformations) is a cruder classification than the LOCC classification. The study of SLOCC classes however yield to strong results that makes LOCC classification also possible in certain cases.

The the characterization of SLOCC classes, however, remains a hard task and is only known for special cases such as few parties with low local dimensions or in the multipartite scenario, for generic states. In applications however one often encounters non-generic states. In this project, we investigate the entanglement properties of a relevant class of non-generic states: the set of normal MPS. We characterize when two normal MPS can be transformed into each other with SLOCC transformations. As the SLOCC operations do not respect translation invariance, we need to use the techniques developed in in Section 3.5 to analyze this setup.

Matrix Product States: Entanglement, symmetries, and state transformations

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We analyze entanglement in the family of translationally-invariant matrix product states (MPS). We give a criterion to determine when two states can be transformed into each other by SLOCC transformations, a central question in entanglement theory. We use that criterion to determine SLOCC classes, and explicitly carry out this classification for the simplest, non-trivial MPS. We also characterize all symmetries of MPS, both global and local (inhomogeneous). We illustrate our results with examples of states that are relevant in different physical contexts.

1. Introduction: Entanglement is a resource for numerous striking applications of quantum information theory [1, 2]. Furthermore, it is key to comprehend many peculiar properties of quantum many-body systems [3, 4] and has become increasingly important in areas like quantum field theory or quantum gravity [5, 6]. Despite its relevance, entanglement is far from being fully understood; at least in the multipartite setting. State transformations play a crucial role as they define a partial order in the set of states. For instance, if a state Ψ can be transformed into a state Φ deterministically by local operations and classical communication (LOCC), then Ψ is at least as entangled as Φ [2]. If two states cannot even probabilistically be interconverted via local operations, i.e., by so-called stochastic LOCC (SLOCC) transformations, their entanglement is not comparable, as one or the other may be more useful for different informational tasks [7]. Thus, the study of state transformations is crucial for the theory of entanglement.

For bipartite systems, state transformations are fully characterized and have led to a very clear picture [8, 9], which is widely used in different areas of research. For more parties such a characterization is much more challenging. In general, there are infinitely many classes of states that can be interconverted via SLOCC, and only in few cases they can be characterized, like for symmetric states or for certain tripartite and four-partite states [10–15]. Moreover, for more than four parties of the same local dimensions almost no state can be transformed into an inequivalent state via deterministic LOCC, and the partial order induced by LOCC becomes trivial [16, 17]. This shows that generic states are not very interesting from the perspective of local transformations. Additionally, most of the states in the Hilbert space cannot be reached in polynomial time even if constant-size nonlocal gates are allowed [18]. Hence, the study of state transformations can be reduced to families of non-generic, but physically relevant states.

In this Letter we present a systematic investigation of state transformations for Matrix Product States (MPS) that describe translationally invariant systems (with periodic boundary conditions) [19, 20]. Ground states of gapped 1D local Hamiltonians or states generated sequentially by a source can be efficiently approximated by MPS [21, 22]. Hence, these states play a very important role in both, quantum information theory and in many-body physics. Despite the fact that they describe a broad variety of phenomena, they have a simple description: tripartite states – the fiducial states of MPS – completely characterize the MPS. We give a criterion to estipulate when an SLOCC transformation between two such MPS exists, and further give criteria to determine the SLOCC classes dictated by such a relation. These classes build a finer structure on top of the SLOCC classification of the fiducial states, with the additional structure depending on the system size.

The methods introduced here also allow us to identify all local symmetries of MPS (not only corresponding to unitary representations [23, 24])[25]. This is interesting on its own right in the theory of tensor networks, as it induces a classification of zero temperature phases of matter [26–28]. As we show, the problems we address can be mapped to finding out certain cyclic structures of operators acting on tripartite states. Thus, our results allow to answer questions like: Can an AKLT state be transformed into a cluster state? What are all the symmetries of these states? What are the SLOCC classes of MPS? As we show, the answers to these questions can be strongly size-dependent.

2. Matrix Product States: We consider here a chain of N d-level systems in a translationally invariant MPS. One such state, $\Psi(A)$, is defined in terms of a tripartite

fiducial state,

$$|A\rangle = \sum_{j=0}^{d-1} \sum_{\alpha,\beta=0}^{D-1} A^j_{\alpha,\beta} |j,\alpha,\beta\rangle \tag{1}$$

as

$$|\Psi(A)\rangle = \sum_{j_1,\ldots,j_N} \mathrm{Tr}(A^{j_1}\ldots A^{j_N})|j_1,\ldots,j_N\rangle. \tag{2}$$

Here, D denotes the bond dimension and A^j a matrix with components $A^j_{\alpha,\beta}$. The corresponding tensor is called *injective* if those matrices span the set of $D\times D$ matrices. The matrix $\mathcal{A} = \sum_{j,\alpha,\beta} A^j_{\alpha,\beta}|j\rangle\langle\alpha,\beta|$ then has a left inverse $\mathcal{A}^{-1}$ [20]. This does not occur generically since it requires that $d \geq D^2$. We consider here *normal* tensors instead, which are generic and are those that become injective after blocking $L \leq 2D^2(6+\log_2(D))$ sites [29]. Furthermore, we consider $N \geq 2L+1$, so that we can apply the fundamental theorem of MPS [30]. We call $\mathcal{N}_{N,D}$ the set of normal, translationally invariant MPS with bond dimension D and $N \geq 2L+1$ sites. Note also that we only consider states with full local ranks as we could otherwise map the problem to smaller local dimensions.

We use several examples of some particularly relevant states of bond dimension 2 to illustrate our results. They are generated by fiducial states $|X_b\rangle = (\mathbb{1}\otimes b\otimes\mathbb{1})|X\rangle$, where X is one of the following states:

(i) the W state $|W\rangle = |100\rangle + |010\rangle + |001\rangle$;
(ii) the GHZ state $|GHZ\rangle = |000\rangle + |111\rangle$;
(iii) the cluster state $|GHZ_H\rangle$, where $H = \sum_{ij}(-1)^{ij}|i\rangle\langle j|$;
(iv) the state $|A_A\rangle = \sqrt{2}|010\rangle - |100\rangle + |111\rangle - \sqrt{2}|201\rangle$, which generates the AKLT state;
(v) the state $|VB\rangle = \sum_{ij}|k_{ij}ij\rangle$ with $d=4$ and $k_{ij} = 2i+j$ generating the valence bond state.

The W and GHZ states play a central role in entanglement theory [12, 31], the cluster state in measurement-based quantum computation [32], and the AKLT [33] and the valence bound state are paradigmatic examples that appear in condensed matter physics. The latter is, furthermore, injective and the fixed point of a renormalization procedure [34].

3. Symmetries: Global symmetries, of the form $S^{\otimes N}$, of MPS were considered in [23, 24], and have led to the classification of phases of MPS in spin chains [26–28]. Here we extend those results in two ways by considering: (i) non-unitary symmetries and (ii) local symmetries for which the operators acting on different spins can be different [25]. That is, given $\Psi(A)\in\mathcal{N}_{N,D}$ we look for all operators $g = \bigotimes_{j=1}^N g_j$ such that $|\Psi(A)\rangle = g|\Psi(A)\rangle$.

In order to solve this problem, we define

$$G_A = \{h = g\otimes x\otimes y^T \mid h|A\rangle = |A\rangle\} \tag{3}$$

where T denotes the transponse in the standard basis. We say that $h_1, h_2 \in G_A$ with $h_i = g_i\otimes x_i\otimes y_i^T$, can be concatenated and write $h_1 \to h_2$ if $y_1x_2 \propto \mathbb{1}$. For $k\in\mathbb{N}$ we call a sequence $\{h_i\}_{i=1}^k \subseteq G_A$ with

$$h_1 \to h_2 \to \ldots \to h_k \to h_1 \tag{4}$$

a $k-$cyle. Then we have:

Theorem 1. *The local (global) symmetries of $\Psi(A)\in\mathcal{N}_{N,D}$ are in one-to-one correspondence with the N-cycles (1-cycles) in G_A.*

The symmetry of the state corresponding to the cycle $h_1\to h_2\to\ldots\to h_N\to h_1$ is $g_1\otimes\cdots\otimes g_N$. The trivial symmetry with $g=\mathbb{1}$ always exists. The proof is based on the fundamental theorem of MPS [30] and is given in the Supplemental Material (SM) [35]. Hence, one simply has to determine G_A and find all of its N-cycles to characterize the local symmetries of $\Psi(A)$. It suffices to find all minimal cycles of G_A from which all others can be obtained by concatenation. For example, a 2-cycle can always be concatenated with itself to an N-cycle if N is even. The global symmetries are defined in terms of 1-cycles, and thus require $g\otimes x^{-1}\otimes x^T|A\rangle = |A\rangle$. For g unitary we therefore recover previous results [23, 24]. The novelty relies on the fact that one may also have local symmetries, with different g_j. In the following we illustrate this fact and the dependence of the symmetries on the system size.

For injective MPS with $D=d^2$ it is straightforward to show that [35]

$$G_A = \{s_{x,y}\otimes x\otimes y^T \mid x,y\in GL(D,\mathbb{C})\}, \tag{5}$$

where $s_{x,y} = \mathcal{A}(x^{T^{-1}}\otimes y^{-1})\mathcal{A}^{-1}$. These operators can be concatenated to infinitely many cycles of arbitrary length. The corresponding symmetries are parametrized via regular matrices $x_1,\ldots,x_N$ as

$$S(x_1,\ldots,x_N) = s_{x_N^{-1},x_1}\otimes\ldots\otimes s_{x_{N-1}^{-1},x_N}. \tag{6}$$

For $\mathcal{A}=\mathbb{1}$ we obtain the large local symmetry group of the injective valence bond state. Normal (but not injective) states have a much smaller set of symmetries. For the AKLT state

$$G_{A_A} = \{s_x\otimes x^{-1}\otimes x^T \mid x\in GL(2,\mathbb{C})\}, \tag{7}$$

where s_x is a function given in the SM [35]. Clearly, elements of G_{A_A} can only be concatenated with themselves. Consequently, the local symmetry group of the AKLT state possesses only global symmetries of the form $s_x^{\otimes N}$. Moreover, this group is isomorphic to the projective linear group $PGL(2,\mathbb{C})$ and includes the well-known symmetries with $s_x\in SO(3)$ [33]. For the AKLT-type states we have $G_{A_{A,g}} = (\mathbb{1}\otimes g\otimes\mathbb{1})G_A(\mathbb{1}\otimes g^{-1}\otimes\mathbb{1})$ and the local symmetries of $\Psi(A_{A,g})$ read

$$S(x) = s_x\otimes s_{g^{-1}xg}\otimes\ldots\otimes s_{g^{-(N-1)}xg^{N-1}}, \tag{8}$$

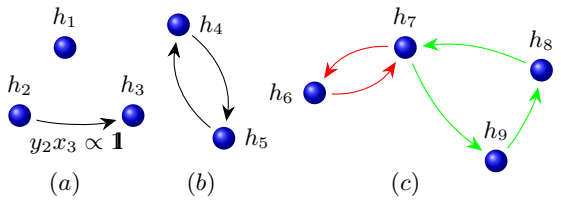

FIG. 1: Graphical representation of how operators in G_A (balls) can be concatenated (edges). (a) h_1 cannot be concatenated, h_2 only with h_3 meaning $y_2x_3 \propto \mathbb{1}$; (b) h_4 and h_5 form a two-cycle; (c) two minimal cycles sharing an operator.

where x is such that $g^{-N}xg^N = x$. Hence, $G_{A_{A,g}}$ is generically smaller than G_{A_A}. Moreover, it consists of non-global symmetries which are N-dependent. The symmetries of the cluster state are also non-global and coincide with the 2^N so-called stabilizer symmetries [35, 36]. For W-generated states the set $G_{A_{W,g}}$ contains infinitely many elements. However, the only nontrivial minimal cycles are 2-cycles. Hence, the corresponding MPS has only the trivial symmetry for odd N and infinitely many non-translationally invariant symmetries for even N.

4. State transformations: Here, we answer the question of when a state, $\Psi(A)$, can be converted into another one, $\Psi(B)$, by SLOCC. As both states correspond to normal tensors, they both belong to $\mathcal{N}_{N,D}$. We write $A \overset{N}{\to} B$ if the transformation is possible. Note that

$$A \overset{N}{\to} B \quad \text{iff} \quad \bigotimes_{j=1}^{N} g_j |\Psi_N(A)\rangle = |\Psi_N(B)\rangle \tag{9}$$

for some g_j. We distinguish also here between global (where all g_j are equal) and local transformations. As for symmetries, we define the set

$$G_{A,B} = \left\{ h = g \otimes x \otimes y^T \mid h|A\rangle = |B\rangle \right\}, \tag{10}$$

where x, y are regular, but not necessarily g. That is, we also consider the case where the physical dimensions, d_A and d_B do not coincide. It is straightforward to show that if $|B\rangle = h_0|A\rangle$ with $h_0 = g_0 \otimes x_0 \otimes y_0^T$ then $G_{A,B} \supseteq h_0 G_A$. For $d_A = d_B$, which is the case iff g_0 is regular, we have $G_{A,B} = h_0 G_A$. Defining concatenations of elements in $G_{A,B}$ as well as k-cycles as before, we have:

Theorem 2. *$A \overset{N}{\to} B$ with local (global) transformations iff there exists an N-cycle (1-cycle) in $G_{A,B}$.*

The proof is given in the SM [35]. Theorem 2 solves the state transformation problem. We can immediately make some simple statements about different possibilities that may occur. For instance, if $G_{A,B}$ only contains a 1-cycle, then $A \overset{N}{\to} B$ for all N with just global transformations. However, if the only minimal cycle is a 2-cycle, then the transformation can only happen for even N. As we illustrate in the following, some transformations might require more sophisticated operations and one obtains a rich variety of situations.

An injective $\Psi(A) \in \mathcal{N}_{N,D}$ can be transformed to any $\Psi(B) \in \mathcal{N}_{N,D}$ via the global operation

$$(\mathcal{B}\mathcal{A}^{-1})^{\otimes N} |\Psi(A)\rangle = |\Psi(B)\rangle. \tag{11}$$

However, using that $G_{A,B} \supseteq (\mathcal{B}\mathcal{A}^{-1} \otimes \mathbb{1} \otimes \mathbb{1}) G_A$, with G_A given in (5), we find that $G_{A,B}$ also contains infinitely many N-cycles that lead to non translationally invariant operators that transform $|\Psi(A)\rangle$ into $|\Psi(B)\rangle$. As a special case, we obtain the well-known result that the injective valence bond state can be transformed to any MPS in $\mathcal{N}_{N,2}$. Since injective MPS are generic in $\mathcal{N}_{N,D}$ for $d = D^2$, a randomly selected MPS of these dimensions can be transformed into any other state of the same dimensions. In contrast to that, transformations from normal (but not injective) states are much more restricted. For example, we show below that for $d = D = 2$ any two randomly selected states $\Psi(A), \Psi(B) \in \mathcal{N}_{N,2}$ cannot be transformed into each other for any N. For the AKLT state and the cluster state, $G_{A_A, A_{Cl}}$ contains only 2-cycles. Hence, the AKLT state can be transformed into the cluster state iff N is even (see SM [35]). The reverse transformation is impossible since the physical dimension cannot be increased. Particularly sophisticated transformations are necessary to transform the AKLT state into certain AKLT-type states, $\Psi(A_{A,g})$, for which

$$G_{A_A, A_{A,g}} = \{ s_x \otimes g x^{-1} \otimes x^T \mid x \in GL(\mathbb{C}, 2) \}.$$

Using Theorem 2 it is easy to show that $A_A \overset{N}{\to} A_{A,g}$ iff $g^N \propto \mathbb{1}$. Hence, the feasibility of this transformation is highly size dependent. Moreover, for any $M \in \mathbb{N}$ there exists a regular g such that $A_A \overset{M}{\to} A_{A,g}$ is not possible for any $M < N$, but it is for $M = N$.

5. Equivalence classes under SLOCC transformations: SLOCC classes give a coarse but very useful classification of entanglement in many-body systems. We show now how these classes can be obtained for $\mathcal{N}_{N,D}$.

We write $A \overset{N}{\sim} B$ if $\Psi(A)$ is SLOCC equivalent to $\Psi(B)$, i.e.,

$$A \overset{N}{\sim} B \quad \text{iff} \quad \bigotimes_{j=1}^{N} g_j |\Psi(A)\rangle = |\Psi(B)\rangle \tag{12}$$

for some regular g_j. Thus, we can reduce the study of SLOCC classes to that of the tripartite fiducial states.

In order to simplify this task, let us make some observations. First, $A \overset{N}{\sim} B$ iff $A \overset{N}{\to} B$ and $B \overset{N}{\to} A$. Because of Theorem 2 the equivalence $A \overset{N}{\sim} B$ thus requires $G_{A,B} \neq \emptyset$ and therefore that $|A\rangle$ and $|B\rangle$ themselves belong to the same tripartite SLOCC class. Hence, the

equivalence relation $\overset{N}{\sim}$ induces a classification that is finer than the SLOCC classification of tripartite states. Second, for any regular g, $g^{\otimes N}|\Psi(A)\rangle$ is obviously in the same class as $|\Psi(A)\rangle$ and for any regular x we trivially have $|A\rangle \overset{N}{\sim} (\mathbb{1}\otimes x^{-1}\otimes x^T)|A\rangle$, since both states correspond to the same MPS. That is, $A \overset{N}{\sim} B$ trivially holds if the relation $|B\rangle = (g\otimes x^{-1}\otimes x^T)|A\rangle$ holds (i.e., there exists a 1-cycle). We get rid of this trivial case by restricting the SLOCC classes to the quotient set induced by that relation. Hence, it only remains to consider states of the form $|A_b\rangle = (\mathbb{1}\otimes b\otimes \mathbb{1})|A\rangle$. This observation leads to the following procedure to characterize SLOCC classes of normal MPS (see Fig. 2): (i) for each tripartite SLOCC class, choose a representative, A; (ii) consider all states $|A_b\rangle = (\mathbb{1}\otimes b\otimes \mathbb{1})|A\rangle$ corresponding to a normal tensor; (iii) determine the classes among those states according to the relation $\overset{N}{\sim}$. We now show how this procedure can be carried out.

According to Theorem 2, $A_b \overset{N}{\sim} A_c$ requires the existence of an N-cycle in G_{A_b,A_c} (or, equivalently, in G_{A_c,A_b}). The fact that $G_{A_b,A_c} = (\mathbb{1}\otimes c\otimes \mathbb{1})G_A(\mathbb{1}\otimes b^{-1}\otimes \mathbb{1})$ motivates the following definition (analogous to (4)). We say that $h_1, h_2 \in G_A$, with $h_i = g_i\otimes x_i\otimes y_i^T$, can be $(b\to c)$-concatenated, if $y_1 b x_2 \propto c$ and then write $h_1 \xrightarrow{b\to c} h_2$. A sequence $\{h_i\}_{i=1}^k \subseteq G_A$ is called a $(b\to c)$-k-cycle if

$$h_1 \xrightarrow{b\to c} h_2 \xrightarrow{b\to c} \ldots \xrightarrow{b\to c} h_k \xrightarrow{b\to c} h_1. \tag{13}$$

We obtain the following corollary to Theorem 2.

Corollary 1. *$A_b \overset{N}{\sim} A_c$ holds nontrivially iff there exists a $(b\to c)$-N-cycle in G_A with $N>1$, but no $(b\to c)$-1-cycle.*

Note that this corollary requires that the N-cycle contains at least two different elements of G_A. This fact can be used to simplify the procedure. For instance, if one wants to determine the A_b connected by 2-cycles, one can take arbitrary α,β and impose $y_\beta b x_\alpha = c \propto y_\alpha b x_\beta$, from which one can eliminate c. Then, the condition can be mapped into the eigenvalue equation $M\vec{b} = \lambda\vec{b}$, where $M = y_\alpha^{-1}y_\beta \otimes (x_\beta^{-1}x_\alpha)^T$. Thus, by choosing all possible pairs in G_A one can identify all classes corresponding to 2-cycles. Corollary 1 solves also straightforwardly the equivalence problem of MPS under local unitary operations (see [34] for global unitary operations).

The procedures above can be carried out whenever the tripartite SLOCC classes are known, as is the case for $d=2, D\geq 2$ [15]. Here, we determine the classes for the simplest non-trivial MPS, i.e., those with $d=D=2$ (see Table I). The fiducial states are either SLOCC equivalent to the GHZ or the W state [12]. Hence, the corresponding SLOCC classes separate into GHZ- and W-generated ones. All W-generated MPS are SLOCC equivalent. As explained before, it, hence, remains to consider states of the form $|GHZ_b\rangle = \mathbb{1}\otimes b\otimes\mathbb{1}|GHZ\rangle$. The resulting classes can be coarse grained into three sets according to the value of $\chi(b) \equiv \frac{b_{00}b_{11}}{b_{01}b_{10}}$, where b_{ij} denote the entries of b: (i) the generic set ($\chi\neq -1,0$); (ii) the cluster set ($\chi=-1$); (iii) the symmetryless set ($\chi=0$). The generic set is of full measure in the set of all MPS with $d=D=2$ and is comprised of states whose local symmetries are of the form $\{\mathbb{1}, s^{\otimes n}\}$. For two such states we have

$$GHZ_b \overset{N}{\sim} GHZ_c \;\Leftrightarrow \chi(b) = \begin{cases} \chi(c) \text{ or } \chi(c)^{-1} & \text{and } N \text{ even} \\ \chi(c) & \text{and } N \text{ odd.}\end{cases}$$

Thus, there are infinitely many, N-dependent classes. The cluster set coincides with the set of states which are SLOCC equivalent to the cluster state. They possess 2^N local symmetries. The states in the symmetryless set are also all SLOCC equivalent and have only the trivial local symmetry. Combined with the class of the non-normal MPS generated by the GHZ state these classes constitute the SLOCC classification of entangled MPS with $d=D=2$.

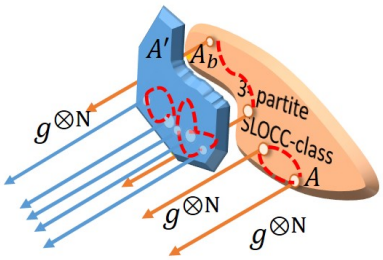

FIG. 2: Illustration of SLOCC classes of MPS in accordance with the procedure given in the main text.

type	χ	# symm.	# SLOCC classes
GHZ	$\neq -1, 0$	2	∞ (see main text)
	-1	2^N	1 (cluster set)
	0	1	1 (symmetryless set)
W	n.a.	N-dependent	1

TABLE I: The SLOCC classification of normal $d=D=2$ MPS. See the SM [35] for more details.

6. Summary and outlook: We solved the problem of when an MPS generated by a normal tensor can be transformed into another via SLOCC and showed how local symmetries of normal MPS can be characterized. In contrast to other results we considered all, in particular non translationally invariant and non unitary, operations. This revealed interesting features of many, particularly relevant states. Furthermore, we provided a procedure to characterize SLOCC classes of normal MPS and explicitly determined them for $d=D=2$. We believe that these results can be extended to non-normal MPS and (certain) Projected Entangled Pair States. Furthermore,

one can also determine the SLOCC classes of MPS with higher dimensions and their corresponding symmetries. The theory presented here also serves as a basis to study deterministic LOCC transformations. Finally, our characterization of all local symmetries may be relevant in the study of phases of matter for 1D systems.

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Supplemental Material

In Section I we first review some properties of MPS that are useful for the remainder of this Supplemental Material (SM). In Section II we proof Theorem 1 and Theorem 2 of the main text. In Section III we determine the local symmetry groups and in Section IV B the transformations of the example states mentioned in the main text. In Section V we derive the SLOCC classification of $d = D = 2$ MPS. We use the same definitions and notations as in the main text. Moreover, we denote by $\sigma_1, \sigma_2, \sigma_3$ the Pauli matrices and use the notation $\mathbb{C}^\times = \mathbb{C} \setminus \{0\}$.

I. INJECTIVE AND NORMAL MATRIX PRODUCT STATES

MPS are defined in terms of rank three tensors. We use the following notation throughout the SM. Let us consider a rank-three tensor $A \in \mathbb{C}^d \otimes \mathbb{C}^D \otimes \mathbb{C}^D$ with

$$A = \sum_{i=0}^{d-1} \sum_{\alpha,\beta=0}^{D-1} A^i_{\alpha\beta} |i\rangle|\alpha\rangle\langle\beta|. \tag{1}$$

Given the tensor A, we write:

$$A^i = \sum_{\alpha\beta} A^i_{\alpha\beta} |\alpha\rangle\langle\beta|, \tag{2}$$

$$|A\rangle = \sum_{i\alpha\beta} A^i_{\alpha\beta} |i\rangle|\alpha\rangle|\beta\rangle, \tag{3}$$

$$\mathcal{A} = \sum_{i\alpha\beta} A^i_{\alpha\beta} |i\rangle\langle\alpha\beta|. \tag{4}$$

Clearly, the last two tensors and the set of matrices $\{A^i\}$ are equivalent representations of A. The state $|A\rangle$ is often referred to as the fiducial state of the tensor. It can also be expressed as

$$|A\rangle = (\mathbb{1} \otimes \mathcal{A} \otimes \mathbb{1}) \left(|\Phi^+\rangle \otimes |\Phi^+\rangle\right) \equiv \mathcal{A}^{(23)} \left(|\Phi^+\rangle \otimes |\Phi^+\rangle\right), \tag{5}$$

where $|\Phi^+\rangle = \sum_{\alpha=0}^{D-1} |\alpha,\alpha\rangle$ is the maximally entangled state.

In this SM, we consider non-translationally invariant (non-TI) MPS on N subsystems that are defined with the help of N different tensors $A_1, \ldots A_N \in \mathbb{C}^d \otimes \mathbb{C}^D \otimes \mathbb{C}^D$ as

$$|\Psi\rangle = \sum_{i_1,\ldots,i_N=0}^{d-1} \mathrm{Tr}\left(A^{i_1}_1 \ldots A^{i_N}_N\right) |i_1,\ldots,i_N\rangle. \tag{6}$$

An MPS that is generated by a single tensor $A = A_1 = \ldots = A_N$ is TI and denoted by $\Psi(A)$.

A particularly important class of MPS is the one which corresponds to *normal* tensors. A set of tensors $A_1, \ldots, A_N$ as defined in Eq. (1) is called normal if there is an L such that any L consecutive tensors satisfy that the map

$$X \mapsto \sum_{i_1,\ldots,i_L=0}^{d-1} \mathrm{Tr}\left(A^{i_1}_k \ldots A^{i_L}_{k+L-1} \cdot X\right) |i_1,\ldots,i_L\rangle \tag{7}$$

is injective. Here and in the following, all indices are periodical, i.e., $i + N \equiv i$. L is referred to as the injectivity length of the MPS. The normality of a tensor can equivalently be characterized as the property that any L consecutive tensors satisfy

$$\operatorname*{span}_{i_1,\ldots,i_L} \left\{A^{i_1}_k \ldots A^{i_L}_{k+L-1}\right\} = \mathbb{C}^{D\times D}. \tag{8}$$

The set of normal MPS on N subsystems with bond dimension D is denoted by $\mathcal{N}_{N,D}$. A tensor is called *injective* if it is normal with $L = 1$. In a slight abuse of standard notation, we call an MPS normal (injective) if the corresponding tensor is normal (injective) respectively. An other equivalent condition for being injective is that the map $\mathcal{A}$ corresponding to the defining tensor A has a left inverse $\mathcal{A}^{-1}$ such that

$$\mathcal{A}^{-1}\mathcal{A} = \sum_{\alpha\beta} |\alpha,\beta\rangle\langle\alpha,\beta|. \tag{9}$$

Note that injectivity requires $d \geq D^2$. Since we are only interested in MPS whose single-subsystem reduced states have full rank the only injective MPS we consider satisfy $d = D^2$.

A fundamental property of MPS is that two different sets of tensors can generate the same state. For instance, if the tensors $B_1, \ldots, B_N$ are related to the tensors $A_1, \ldots, A_N$ as $A_k^j = x_k^{-1} B_k^j x_{k+1}$ for all k, j, with $x_{N+1} \equiv x_1$, then

$$\sum_{i_1,\ldots,i_N=0}^{d-1} \mathrm{Tr}\left(A_1^{i_1} \ldots A_N^{i_N}\right) |i_1, \ldots, i_N\rangle = \sum_{i_1,\ldots,i_N=0}^{d-1} \mathrm{Tr}\left(B_1^{i_1} \ldots B_N^{i_N}\right) |i_1, \ldots, i_N\rangle. \tag{10}$$

For normal tensors, in fact, this is the only way how two different sets of tensors can generate the same states as stated by the fundamental theorem which was proven in Ref. [1]:

Theorem I.1 ([1]). *The tensors $A_1, \ldots, A_N$ and $B_1, \ldots, B_N$ generate the same normal MPS Ψ iff there exist regular matrices $x_1, \ldots, x_N$ such that $A_k^j = x_k^{-1} B_k^j x_{k+1}$ for all k and j, with $x_{N+1} \equiv x_1$; that is, iff*

$$|A_k\rangle = \mathbb{1} \otimes x_k^{-1} \otimes x_{k+1}^T |B_k\rangle \ \forall \ k. \tag{11}$$

The matrices $x_1, \ldots, x_N$ are unique up to a multiplicative constant.

Theorem I.1 is the basis of the proofs of Theorem 1 and Theorem 2 of the main text.

II. PROOF OF THEOREM 1 AND THEOREM 2

In this section we provide the proof of Theorem 1 and Theorem 2 of the main text. To this end, the following Lemma will be important.

Lemma II.1. *Suppose $\Psi \in \mathcal{N}_{N,D}$ defined by a tensor A with injectivity length L can also be written as a MPS with non-TI tensors $B_1, \ldots B_N$, all with bond dimension D. Then this description is also normal with injectivity length L.*

Proof. The two different ways to express the MPS are the following:

$$|\Psi\rangle = \sum_i \mathrm{Tr}(A^{i_1} \ldots A^{i_N}) |i_1 \ldots i_N\rangle = \sum_i \mathrm{Tr}(B_1^{i_1} \ldots B_N^{i_N}) |i_1 \ldots i_N\rangle. \tag{12}$$

Let us apply any linear functional to the last $N-k$ subsystems, where k satisfies $L \leq k \leq N-L$. That is, we consider the vector space

$$V = \left\{ \sum_i f_{i_{k+1} \ldots i_N} \cdot \mathrm{Tr}(A^{i_1} \ldots A^{i_k} A^{i_{k+1}} \ldots A^{i_N}) |i_1 \ldots i_k\rangle \ \middle| \ f \in \mathbb{C}^{d(N-k)} \right\}. \tag{13}$$

Due to the normality of the A tensor, the products of the last $N-k \geq L$ matrices describing the MPS span the whole space of $D \times D$ matrices, that is,

$$\left\{ \sum_i f_{i_{k+1} \ldots i_N} \cdot A^{i_{k+1}} \ldots A^{i_N} \ \middle| \ f \in \mathbb{C}^{d(N-k)} \right\} = \mathbb{C}^{D \times D}. \tag{14}$$

Therefore, the vector space V can also be written as

$$V = \left\{ \sum_i \mathrm{Tr}(A^{i_1} \ldots A^{i_k} \cdot X) |i_1 \ldots i_N\rangle \ \middle| \ X \in \mathbb{C}^{D \times D} \right\}. \tag{15}$$

Due to the normality of the tensor A, the map

$$X \mapsto \sum_i \mathrm{Tr}(A^{i_1} \ldots A^{i_k} \cdot X) |i_1 \ldots i_N\rangle \tag{16}$$

is injective. As it is also linear, the vector space V is D^2 dimensional. V can also be expressed with the help of the B tensors. Similarly to the derivation above, we find

$$V = \left\{ \sum_i \mathrm{Tr}(B_1^{i_1} \ldots B_k^{i_k} \cdot X) |i_1 \ldots i_N\rangle \ \middle| \ X \in W \leq \mathbb{C}^{D \times D} \right\}, \tag{17}$$

where W is a subspace of the space of all D-by-D matrices that is spanned by the products of the last $N-k$ matrices describing the MPS. As V is D^2 dimensional, it immediately follows that $W = \mathbb{C}^{D\times D}$ and that the map

$$X \mapsto \sum_i \mathrm{Tr}(B_1^{i_1} \dots B_k^{i_k} \cdot X)|i_1 \dots i_N\rangle \tag{18}$$

is injective. This argument can be repeated to any L consecutive subsystems, thus the tensors $B_1, \dots B_N$ form a normal description of the MPS Ψ. □

Using Lemma II.1 we can proof Theorem 1 of the main text, which provides a characterization of the local symmetries of a normal MPS $\Psi(A)$, i.e., of all $S = s_1 \otimes \dots \otimes s_N$ such that

$$S|\Psi(A)\rangle = |\Psi(A)\rangle. \tag{19}$$

We restate the theorem here for the sake of readability.

Theorem 1. *The local (global) symmetries of $\Psi(A) \in \mathcal{N}_{N,D}$ are in one-to-one correspondence with the N-cycles (1-cyles) in G_A.*

Proof. We first show that the $S = s_1 \otimes \dots \otimes s_N$ that solve Eq. (19) correspond to N-cycles in G_A. Note that the state $S|\Psi(A)\rangle$ is an MPS with bond dimension D, generated by the fiducial states $|A_k\rangle = s_k \otimes \mathbb{1} \otimes \mathbb{1}|A\rangle$ for $k = 1, \dots, N$. Lemma II.1 implies that the representation $S|\Psi(A)\rangle$ of the normal MPS $|\Psi(A)\rangle$ is normal too and thus Theorem I.1 can be used to find all S that satisfy Eq. (19). Because of Theorem I.1, Eq. (19) is fulfilled iff there are (up to a multiplicative factor) unique regular matrices $x_1, \dots, x_N$ such that

$$(s_k \otimes x_k^{-1} \otimes x_{k+1}^T)|A\rangle = |A\rangle \ \forall k, \tag{20}$$

where $x_{N+1} = x_1$. That is, $S = s_1 \otimes \dots \otimes s_N$ is a symmetry of $\Psi(A)$ iff there are operators $h_1, \dots, h_N \in G_A$, with $h_k = s_k \otimes x_k \otimes y_k^T$ [2], that can be connected to an N-cycle, i.e., for which $y_k x_{k+1} \propto \mathbb{1}$ holds. This shows that the local symmetry group of $\Psi(A)$ is in one-to-one correspondence with the N-cycles in G_A.

If $S = s^{\otimes N}$ is a global symmetry, $s_k \propto s$ holds and thus the uniqueness (up to a multiplicative factor) of the x_k matrices in Eq. (20) implies that they are all proportional to each other. Hence, a symmetry is global iff it originates from a 1-cycle. □

Theorem 2 provides a criterion for when the transformation $A \overset{N}{\to} B$ is possible, i.e., when there is a $g = g_1 \otimes \dots \otimes g_n$ such that

$$g|\Psi(A)\rangle = |\Psi(B)\rangle. \tag{21}$$

We again restate the theorem before we prove it.

Theorem 2. *$A \overset{N}{\to} B$ with local (global) transformations iff there exists an N-cycle (1-cycle) in $G_{A,B}$.*

Proof. The "if"-part is trivial. To prove the "only if"-part suppose that Eq. (21) holds. Then $g|\Psi(A)\rangle$ is an MPS representation of $\Psi(B)$ with the same bond dimensions. Lemma II.1 then implies that $g|\Psi(A)\rangle$ is normal too; even if g is singular. Hence, $g|\Psi(A)\rangle$ and $\Psi(B)$ have to be related as stated by the fundamental theorem, Theorem I.1. Analogously to the proof of Theorem 1 one can use this to show that g has to correspond to an N-cycle in $G_{A,B}$. □

III. SYMMETRIES OF EXAMPLES IN THE MAIN TEXT

In this section we derive the symmetries of the states presented in the main text. We denote the local symmetry group of $\Psi(A)$ by

$$S_{\Psi(A)} \equiv \{S = s_1 \otimes \dots \otimes s_N \mid S|\Psi(A)\rangle = |\Psi(A)\rangle\}. \tag{22}$$

A. Symmetries of injective MPS

For injective MPS we use decomposition (5) for the fiducial state and the fact that $\mathcal{A}^{-1}$ exists if the MPS is injective. Moreover, we use that the maximally entangled state defined after Eq. (5) satisfies the following equation for any x,

$$(\mathbb{1}\otimes x)|\Phi^+\rangle = (x^T\otimes\mathbb{1})|\Phi^+\rangle. \tag{23}$$

Using these properties it is straightforward to verify that

$$G_A = \{s_{x,y}\otimes x\otimes y^T | x,y\in GL(D,\mathbb{C})\}, \tag{24}$$

where $s_{x,y} = \mathcal{A}(x^{T^{-1}}\otimes y^{-1})\mathcal{A}^{-1}$. Clearly, the symmetry $s_{x,y}\otimes x\otimes y^T$ can be connected to any symmetry $s_{y^{-1},z}\otimes y^{-1}\otimes z^T$, where $z\in GL(D,\mathbb{C})$ is arbitrary. Using this in combination with Theorem 1 yields

$$S_{\Psi(A)} = \left\{ s_{x_N^{-1},x_1}\otimes\ldots\otimes s_{x_{N-1}^{-1},x_N}\right\}_{x_1,\ldots,x_N\in GL(D,\mathbb{C})}. \tag{25}$$

B. Symmetries of the AKLT state

The AKLT state is generated by the matrices [3]

$$A_A^0 = \sqrt{2}\begin{pmatrix}0&0\\1&0\end{pmatrix},\ A_A^1 = \begin{pmatrix}-1&0\\0&1\end{pmatrix},\ A_A^2 = \sqrt{2}\begin{pmatrix}0&-1\\0&0\end{pmatrix}. \tag{26}$$

We use that

$$s\otimes x\otimes y^T\in G_{A_A}\ \Leftrightarrow\ xA_A^i y = \sum_{j=0}^{2}(s^{-1})_{ij}A_A^j\ \forall i, \tag{27}$$

where $(s^{-1})_{ij}$ denotes the entries of s^{-1}. We can then take the trace on the right-hand side of Eq. (27) and use that the matrices A_A^j are traceless to obtain the following equation,

$$\mathrm{Tr}(A_A^i yx) = \sum_j (s^{-1})_{ij}\mathrm{Tr}(A_A^j) = 0\ \forall i. \tag{28}$$

Note further that $(\mathbb{1}, A_A^0, A_A^1, A_A^2)$ forms an orthogonal basis of all 2-by-2 matrices. Thus, Eq. (28) implies that $y = \frac{1}{\lambda}x^{-1}$ for some $\lambda\neq 0$. Inserting this into the right-hand side of (27) yields

$$xA_A^i x^{-1} = \lambda\sum_j (s^{-1})_{ij}A_A^j \tag{29}$$

We can absorb λ in the definition of s and thus set $\lambda = 1$, without loss of generality. Since (A_A^0, A_A^1, A_A^2) is a basis of all traceless 2-by-2 matrices one can then find, for any regular x, a regular $s = s_x$ such that Eq. (29) holds. Summarizing, this shows that $G_A = \{s_x\otimes x^{-1}\otimes x^T\}_{x\in GL(2,\mathbb{C})}$. Using Theorem 1 then further shows that

$$S_{\Psi(A_A)} = \left\{s_x^{\otimes N}\right\}_{x\in GL(2,\mathbb{C})}. \tag{30}$$

Note that the following observation holds.

Observation III.1. *The symmetry group $S_{\Psi(A_A)}$ is isomporphic to the projective linear group $PGL(2,\mathbb{C})$.*

Proof. We have to show that the following is satisfied for any regular x, y

$$s_x = s_y \Leftrightarrow x\propto y. \tag{31}$$

From Eq. (29) (recall that we have set, w.l.o.g., $\lambda = 1$) it is easy to see that $x\propto y$ implies $s_x = s_y$. To show that also the reverse holds suppose that $s_x = s_y$ holds for some regular x, y. Then Eq. (29) (again with $\lambda = 1$) implies that $xA_A^i x^{-1} = yA_A^i y^{-1}$ for all i, which is equivalent to

$$y^{-1}xA_A^i = A_A^i y^{-1}x\ \forall i. \tag{32}$$

This shows that $y^{-1}x$ commutes with all A_A^i. Since $(\mathbb{1}, A_A^0, A_A^1, A_A^2)$ forms a basis of all 2-by-2 matrices this shows that $y^{-1}x\propto\mathbb{1}$. □

C. Symmetries of AKLT-type states

The AKLT-type states are generated by the fiducial state $|A_{A,g}\rangle = (\mathbb{1}\otimes g\otimes \mathbb{1})|A_A\rangle$, where $g \in GL(2,\mathbb{C})$ is such that the resulting state is normal. As noted in the main text we have

$$G_{A_{A,g}} = (\mathbb{1}\otimes g\otimes \mathbb{1})\cdot G_A \cdot (\mathbb{1}\otimes g^{-1}\otimes \mathbb{1}) = \{h_x \equiv s_x \otimes g x^{-1} g^{-1} \otimes x^T\}_{x\in GL(2,\mathbb{C})}. \tag{33}$$

Two operators $h_x, h_y \in G_{A_{A,g}}$ can be concatenated iff $y \propto g^{-1}xg$. Hence, the operators $h_{x_1},\ldots,h_{x_N}$ form an N-cycle iff

$$x_{k+1} \propto g^{-1}x_k g \;\forall k \tag{34}$$

where $x_{N+1}\equiv x_1$. This is fulfilled for an $x\equiv x_1$ iff $x = g^{-N}xg^N$. Using Theorem 1 this yields

$$S_{\Psi(A_{A,g})} \equiv \{s_x \otimes s_{g^{-1}xg}\otimes\ldots\otimes s_{g^{-(N-1)}xg^{N-1}} \mid x\in GL(2,\mathbb{C}), x = g^{-N}xg^N\}. \tag{35}$$

D. Cluster state and W-generated states

We refer the reader to Section V, where we characterize the SLOCC classes and the local symmetries of all normal MPS with $d = D = 2$.

IV. TRANSFORMATIONS OF EXAMPLES IN THE MAIN TEXT

In this section we derive the transformations of the states presented in the main text.

A. From Injective MPS to other MPS

We again use decomposition (5) and the fact that $\mathcal{A}^{-1}$ exists for injective MPS. For an injective MPS $\Psi(A)\in\mathcal{N}_{N,D}$ and an arbitrary $\Psi(B)\in\mathcal{N}_{N,D}$ it is then straightforward to see that $(\mathcal{B}\mathcal{A}^{-1}\otimes\mathbb{1}\otimes\mathbb{1})\in G_{A,B}$ forms a 1-cycle and thus the transformation $A \overset{N}{\to} B$ can be achieved via a global operation as

$$(\mathcal{B}\mathcal{A}^{-1})^{\otimes N}|\Psi(A)\rangle = |\Psi(B)\rangle. \tag{36}$$

Combining Theorem 1 with the fact that $G_{A,B} = (\mathcal{B}\mathcal{A}^{-1}\otimes\mathbb{1}\otimes\mathbb{1})\cdot G_A$, where G_A is given in Eq. (24), it is easy to see that there are also infinitely many non-TI operations that achieve the transformation $A\overset{N}{\to}B$.

B. From the AKLT state to the cluster state

Let us now determine when the AKLT state can be transformed into the cluster state. The cluster state is generated by the fiducial state $|A_{Cl}\rangle = (\mathbb{1}\otimes H\otimes\mathbb{1})|GHZ\rangle$, where $H = \sum_{i,j=0}^{1}(-1)^{ij}|i\rangle\langle j|$ and $|GHZ\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ is the three-qubit GHZ state. Note that we can write

$$G_{A_A,A_{Cl}} = (\mathbb{1}\otimes H\otimes\mathbb{1})\cdot G_{A_A,GHZ}. \tag{37}$$

Let us first determine $G_{A_A,GHZ}$. To this end, note that $G_{A_A,GHZ}\subset\mathbb{C}^{2\times3}\otimes GL(2,\mathbb{C})\otimes GL(2,\mathbb{C})$, where we have used that A_A and the GHZ state are both tripartite entangled and, therefore, the operators on the bond dimensions have to be invertible. Note further that any $x\in\mathbb{C}^{2\times3}$ can be expressed as $x = zM$, where $z\in GL(2,\mathbb{C})$ and M is a 2-by-3 matrix in reduced row-echelon form [4], i.e., is an element of the set

$$E_{2,3} \equiv \left\{M_1(\alpha,\beta)\equiv\begin{pmatrix}1&0&\alpha\\0&1&\beta\end{pmatrix}\right\}_{\alpha,\beta\in\mathbb{C}} \cup \left\{M_2\equiv\begin{pmatrix}1&0&0\\0&0&1\end{pmatrix},\ M_3\equiv\begin{pmatrix}0&1&0\\0&0&1\end{pmatrix}\right\}. \tag{38}$$

Hence, we can write $h\in G_{A_A,GHZ}$ as $h = w(M\otimes\mathbb{1}\otimes\mathbb{1})$, where $w\in GL(2,\mathbb{C})^{\otimes3}$ and $M\in E_{2,3}$. A necessary condition for $h\in G_{A_A,GHZ}$ obviously is that $h|A_A\rangle$ is a state in the SLOCC class of the GHZ state. Recall that a general

three-qubit state $|\psi\rangle = |0\rangle|\phi_0\rangle + |1\rangle|\phi_1\rangle$, with $|\phi_i\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$, is an element of the GHZ class iff its three-tangle is non-vanishing [5], i.e., iff

$$\tau_3(\psi) = \left|\det \begin{pmatrix} \langle\phi_0^*|\sigma_2^{\otimes 2}|\phi_0\rangle & \langle\phi_0^*|\sigma_2^{\otimes 2}|\phi_1\rangle \\ \langle\phi_1^*|\sigma_2^{\otimes 2}|\phi_0\rangle & \langle\phi_1^*|\sigma_2^{\otimes 2}|\phi_1\rangle \end{pmatrix}\right| \neq 0. \tag{39}$$

Here, $|\phi^*\rangle$ denotes the complex conjugate of the state $|\phi\rangle$ in the computational basis. Moreover, for any $t \in GL(2,\mathbb{C})^{\otimes 3}$ we have that $\tau(t|\psi\rangle) \neq 0$ iff $\tau(\psi) \neq 0$.

Hence, $h = w(M \otimes \mathbb{1} \otimes \mathbb{1}) \in G_{A_A,GHZ}$ has to fulfill

$$\tau(M \otimes \mathbb{1} \otimes \mathbb{1}|A_A\rangle) \neq 0. \tag{40}$$

Inequality (40) is satisfied iff $M = M_1(\alpha,\beta)$ with $\alpha \neq -\frac{\beta^2}{2}$ or $M = M_2$. In particular, it is not fulfilled for $M = M_3$, such that we no longer have to consider this case. For matrices M that fulfill inequality (40) it is straightforward to find a $w \in GL(2,\mathbb{C})^{\otimes 3}$ such that $h = w(M \otimes \mathbb{1} \otimes \mathbb{1}) \in G_{A_A,GHZ}$. In this way, we arrive at the following operators of $G_{A_A,GHZ}$,

$$h_1(\alpha,\beta) = a(\alpha,\beta)M_1(\alpha,\beta) \otimes b(\alpha,\beta) \otimes c(\alpha,\beta), \text{ for } \alpha \neq -\frac{\beta^2}{2}, \tag{41}$$

$$h_2 = M_2 \otimes \sigma_1 \otimes \mathbb{1}, \tag{42}$$

where

$$a(\alpha,\beta) \equiv \begin{pmatrix} 1 & -\beta - \sqrt{\beta^2 - 2\alpha} \\ 1 & -\beta + \sqrt{\beta^2 - 2\alpha} \end{pmatrix},$$

$$b(\alpha,\beta) \equiv \begin{pmatrix} -\frac{\sqrt{6}}{4\beta^2 - 8\alpha} & \frac{\sqrt{3}}{4}\frac{\beta - \sqrt{\beta^2-2\alpha}}{2\alpha - \beta^2} \\ 1 & \frac{1}{\sqrt{2}}(\beta + \sqrt{\beta^2 - 2\alpha}) \end{pmatrix},$$

$$c(\alpha,\beta) \equiv \begin{pmatrix} \frac{1}{\sqrt{2}}(-\beta + \sqrt{\beta^2 - 2\alpha}) & 1 \\ \frac{\sqrt{3}}{4}\frac{\beta - \sqrt{\beta^2-2\alpha}}{2\alpha - \beta^2} & -\frac{\sqrt{6}}{4\beta^2 - 8\alpha} \end{pmatrix}.$$

We obtain the whole set $G_{A_A,GHZ}$ by multiplying these operators from the left with the local symmetry group of the GHZ state, which reads [6]

$$G_{GHZ} = \left\{ s_{GHZ}^{(i,x,y)} = \sigma_1^i P_{\frac{1}{xy}} \otimes \sigma_1^i P_x \otimes \sigma_1^i P_y \right\}_{(i,x,y) \in \{0,1\} \times \mathbb{C}^{\times 2}}, \tag{43}$$

with $P_z = \mathrm{diag}(z, 1/z)$. Combining this with Eq. (37) we obtain,

$$G_{A_A,A_{Cl}} = G^{(1)}_{A_A,Cl} \cup G^{(2)}_{A_A,Cl}, \tag{44}$$

with

$$G^{(1)}_{A_A,Cl} = (\mathbb{1} \otimes H \otimes \mathbb{1}) \cdot G_{GHZ} \cdot \left\{ h_1(\alpha,\beta) \mid \alpha \neq -\frac{\beta^2}{2} \right\}, \; G^{(2)}_{A_A,Cl} = (\mathbb{1} \otimes H \otimes \mathbb{1}) \cdot G_{GHZ} \cdot h_2. \tag{45}$$

Due to Theorem 2 it now only remains to determine the cycles that can be obtained by concatenating elements of $G_{A_A,A_{Cl}}$. It is straightforward to see that elements of $G^{(k)}_{A_A,A_{Cl}}$, for $k \in \{1,2\}$, cannot be concatenated with each other. However, an element of $G^{(1)}_{A_A,A_{Cl}}$ can be concatenated with an element of $G^{(2)}_{A_A,A_{Cl}}$ to form a 2-cycle. The only way to obtain an N-cycle is therefore to alternatingly concatenate elements from $G^{(1)}_{A_A,A_{Cl}}$ and $G^{(2)}_{A_A,A_{Cl}}$; which is possible iff N is even. This proves that $A_A \xrightarrow{N} A_{Cl}$ iff N is even.

Let us note that the method presented here can also be used to determine *all* MPS with $d = D = 2$ to which the AKLT state can be transformed.

C. From the AKLT state to AKLT-type states

Let us determine when the transformation $A_A \overset{N}{\to} A_{A,g}$ from the AKLT state to an AKLT-type state is possible. Note first that

$$G_{A_A,A_{A,g}} = (\mathbb{1}\otimes g\otimes \mathbb{1})\cdot G_{A_A} = \{h_x = s_x\otimes gx^{-1}\otimes x^T | x\in GL(2,\mathbb{C}\}, \tag{46}$$

where s_x was defined in Section III C. The operators $h_{x_1},\ldots,h_{x_N}$ form an N-cycle iff

$$x_{k+1}\propto x_k g\ \forall k, \tag{47}$$

where $x_{N+1}\equiv x_1$. This is fulfilled for any x_1 iff $g^N\propto\mathbb{1}$. Using Theorem 1 we see that the following holds.

$$A_{A_A}\overset{N}{\to} A_{A,g}\ \Leftrightarrow\ g^N\propto\mathbb{1} \tag{48}$$

V. SYMMETRIES AND SLOCC CLASSIFICATION FOR MPS WITH $d = D = 2$

It is straightforward to show that MPS generated by (bi-)separable three-qubit states are product states (i.e. they have bond dimension $D = 1$). Hence, we only have to consider MPS generated by genuinely tripartite entangled three-qubit states, which are either an element of the GHZ class or the W class [7]. As explained in the main text, it is sufficient to determine when normal MPS generated by fiducial states of the form

$$|GHZ_b\rangle = \mathbb{1}\otimes b\otimes\mathbb{1}|GHZ\rangle,\ \text{i.e., with matrices } A^0_{GHZ,b} = b|0\rangle\langle 0|,\ A^1_{GHZ,b} = b|1\rangle\langle 1|,\ \text{or} \tag{49}$$

$$|W_b\rangle = \mathbb{1}\otimes b\otimes\mathbb{1}|W\rangle,\ \text{i.e., with matrices } A^0_{W,b} = b(|0\rangle\langle 1| + |1\rangle\langle 0|),\ A^1_{W,b} = b|0\rangle\langle 0|, \tag{50}$$

are related via transformations that are not global. The whole classification is obtained by adding the states that are related to those states via global operations.

In order to characterize the local symmetry group of all normal MPS (see Eq. (22)) we can use the following property. For $A\overset{N}{\sim}B$ there exists, by definition, an invertible local operator g such that $|\Psi(B)\rangle = g|\Psi(A)\rangle$ and it is straightforward to see that

$$S_{\Psi(B)} = gS_{\Psi(A)}g^{-1}. \tag{51}$$

Hence, it is sufficient to find the symmetries of one representative of an SLOCC class, $\Psi(A)$. Concretely, this means that it is sufficient to characterize the symmetries of MPS of the form (49 - 50).

In order to find the symmetries and SLOCC classes of these MPS we proceed in three steps:

1. Determine for which b the state $\Psi(X_b)$ is normal.
2. Characterize the symmetries of the normal MPS using Theorem 1.
3. Characterize the SLOCC classes of the states $\Psi(X_b)$ using Corollary 1 of the main text. To simplify this procedure, we can use that MPS with different injectivity lengths cannot be SLOCC equivalent (this follows from Lemma II.1). Moreover, MPS whose symmetry groups are not conjugate to each other, i.e., do not fulfill Eq. (51) for some g, can also never be SLOCC equivalent.

The resulting symmetry characterization and SLOCC classification is concisely summarized in Table I, which is an extended version of Table I in the main text. Let us note here that $\Psi(GHZ_{\mathbb{1}}) = |GHZ_N\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle^{\otimes N} + |1\rangle^{\otimes N})$ is the N-qubit GHZ state. This state is not normal and thus the methods of the main text do not directly apply to it. However, the symmetries of GHZ_N are known [6]. Moreover, we show below that all non-normal multipartite entangled MPS are SLOCC equivalent to GHZ_N. Although the SLOCC and symmetry classification of general non-normal MPS is not within the scope of the main text, we could thus determine it for the special case of $d = D = 2$. Combined with the results on normal MPS we therefore obtain here a characterization of the symmetries and SLOCC classes of all multipartite entangled MPS with $d = D = 2$.

In the following we provide a detailed presentation and derivation of these results. We first consider the GHZ- (Section V A) and then the W-generated states (Section V B).

type	# symmetries	inj. length	# SLOCC classes	$A \overset{N}{\sim} B$
GHZ	2	2	∞ (generic set)	$GHZ_b \overset{N}{\sim} GHZ_c \Leftrightarrow \chi(b) = \begin{cases} \chi(c) \text{ or } \chi(c)^{-1}, & N \text{ even} \\ \chi(c), & N \text{ odd.} \end{cases}$
	2^N	2	1 (cluster set)	always
	1	3	1 (symmetryless set)	always
	∞	not normal	1 (GHZ_N class)	always
W	1 for odd N ∞ for even N	2	1	always

Table I. The SLOCC classification of MPS with $d = D = 2$. First, according to the SLOCC class of the generating three-qubit state. For GHZ-generated states one can further coarse grain the classes according to their local symmetries into different sets. We also provide the minimal number of qubits that have to be blocked to make the normal states injective. The only multipartite entangled non-normal states are all SLOCC equivalent to the non-normal state generated by the three-qubit GHZ state, i.e., they are elements of the GHZ_N class. We state how many different SLOCC classes there are within one set and depict when two MPS within this set are SLOCC equivalent. The function χ is defined in Eq. (54) (see also main text). Note that the class with two local symmetries is of full measure in the set of all MPS with $d = D = 2$.

A. GHZ-generated MPS

1. Characterization of the normal MPS

We first determine when $\Psi(GHZ_b)$ is normal, where $b = (b_{ij}) \in GL(2, \mathbb{C})$. That is, we have to check for which $b \in GL(2, \mathbb{C})$ there is an L such that

$$\operatorname*{span}_{i_1,\ldots,i_L} \left\{ A^{i_1}_{GHZ,b} \cdot \ldots \cdot A^{i_L}_{GHZ,b} \right\} = \mathbb{C}^{2\times 2}. \tag{52}$$

Here, we determine the minimal L with this property, i.e., the injectivity length of $\Psi(W_b)$. It is straightforward to see that we have to distinguish four different cases:

(i) $b_{ij} \neq 0$ for all i, j: $L = 2$ and thus the MPS is normal for $N \geq 5$. Note that the states related to MPS of this case via (trivial) global operations are generated by fiducial states of the form $g \otimes x^{-1} b \otimes x^T |GHZ\rangle$ (as shown in the main text), where g, x are arbitrary regular matrices. Since b is a generic regular matrix (for this case) these fiducial states comprise a generic set of three-qubit states. Hence, the MPS corresponding (up to global operations) to this case are generated by a full measure set of three-qubit states and are thus of full measure in the set of all MPS with $d = D = 2$.

(ii) exactly one entry of b is zero:

(iia) $b_{kk} = 0$ for exactly one $k \in \{0, 1\}$: $L = 3$ and thus the MPS is normal for $N \geq 7$,

(iib) $b_{01} = 0$ or $b_{10} = 0$: The MPS is not normal for any N and SLOCC equivalent to $|GHZ_N\rangle$.

(iii) exactly two entries of b are zero: The MPS is either SLOCC equivalent to $|GHZ_N\rangle$ or vanishes and is therefore not normal.

In particular, this shows that normal GHZ-generated MPS have an injectivity length of at most 3 (in case (iia)) and generically (i.e., in case (iiia)) of 2. This is considerably below the best known upper bound (to the knowledge of the authors) of $L \leq 2D^2(6 + \log_2(D))$ for the injectivity length of a normal MPS with physical dimension d and bond dimension D [8]. For $D = 2$ this bound states $L \leq 56$.

2. Characterization of the local symmetries

In the following we determine the local symmetries of the normal GHZ-generated MPS determined before (i.e., of states belonging to the cases (i) and (iia) in the last section). Note that the symmetries of the three-qubit GHZ state are given in Eq. (43). The stabilizer of the GHZ-type state $|GHZ_b\rangle = \mathbb{1} \otimes b \otimes \mathbb{1} |GHZ\rangle$ hence reads

$$G_{GHZ_b} = \left\{ s^{(k,x,y)} = (\mathbb{1} \otimes b \otimes \mathbb{1}) s^{(k,x,y)}_{GHZ} (\mathbb{1} \otimes b^{-1} \otimes \mathbb{1}) \right\}_{(k,x,y) \in \{0,1\} \times \mathbb{C}^\times}.$$

Two elements $s^{(k,v,w)}, s^{(l,x,y)} \in G_{GHZ_b}$ can be concatenated iff

$$P_w \sigma_1^k b \sigma_1^l P_x b^{-1} = r\mathbb{1}, \tag{53}$$

for some $r \neq 0$, where $P_z = \mathrm{diag}(z, 1/z)$. This condition is extremely restrictive and it is easy to find the minimal cycles in G_{GHZ_b} entailed by it. We can simply read off the resulting symmetries (as explained in the main text). This yields the following stabilizer for the cases (i) and (iia) found in Section V A 1.

(i) In solving Eq. (53) the function

$$\chi(b) = \frac{b_{00} \cdot b_{11}}{b_{01} \cdot b_{10}}. \tag{54}$$

plays a prominent role. More precisely, χ can be used to further distinguish the MPS in this case according the following subcases:

(ia) $\chi(b) \neq -1, 0$: Then Eq. (53) only has solutions if $k = l$ and they depend on b. For $k = l = 0$ we get $w = x = \pm 1$. For $k = l = 1$ we get $w^2 = \frac{b_{00} b_{01}}{b_{10} b_{11}}$ and $x = \frac{b_{10}}{b_{01}} w$, $r = 1$. There is only one nontrivial cycle in G_{GHZ_b}, which has length 1. Hence, besides the trivial symmetry, the state $\Psi(GHZ_b)$ has one nontrivial symmetry and its stabilizer reads

$$S_{\Psi(GHZ_b)} = \left\{ \mathbb{1}^{\otimes N}, \left(\sigma_1 P_{\frac{b_{11}}{b_{00}}} \right)^{\otimes N} \right\}, \tag{55}$$

for $N \geq 5$.

(ib) $\chi(b) = -1$: Equation (53) has the following solutions: $r = w = x = 1$ for $k = l = 0$; $r = i, w = i, x = \frac{b_{00}}{b_{01}}$ for $k = 0, l = 1$; $r = i, w = \frac{b_{00}}{b_{10}}, x = 1$ for $k = 1, l = 0$; $r = 1, w = \frac{i b_{00}}{b_{10}}, x = \frac{b_{10}}{b_{01}}$ for $k = l = 1$. Hence, there are many ways to connect elements in G_{GHZ_b}. They give rise to 2^N different N-cycles that each lead to a local symmetry of $|\Psi(GHZ_b)\rangle$. Note that the linear cluster state (with periodic boundary conditions) reads $|Cluster\rangle \equiv |\Psi(GHZ_H)\rangle$, where $H = \sum_{i,j=0}^{1} (-1)^{ij} |i\rangle\langle j|$. For the cluster state we find that the local symmetries are exactly given by its stabilizer symmetries [9], i.e.,

$$S_{Cluster} = S_{\Psi(GHZ_H)} = \left\{ K_1^{i_1} \cdot \ldots \cdot K_N^{i_N} \right\}_{i_1, \ldots, i_N \in \{0,1\}}. \tag{56}$$

Here, $K_i = \sigma_3^{(i-1)} \sigma_1^{(i)} \sigma_3^{(i+1)}$ acts as σ_1 on qubit i and as σ_3 on qubits $i-1, i$ (with periodic boundary conditions) and as the identity on all other qubits. In fact, we see in Section V A 3 below that all states with $\chi(b) = -1$ are SLOCC equivalent, such that we call this set of states the *cluster set*. The symmetries of all states in this set can thus also be easily obtained from the symmetries (56) of the cluster state via Eq. (51).

(iia) These states fulfill $\chi(b) = 0$. There only exists a solution of Eq. (53) for $k = l = 0$ and $w, x = \pm 1$. This results in a trivial stabilizer, i.e.,

$$S_{\Psi(GHZ_b)} = \{\mathbb{1}\}, \tag{57}$$

for $N \geq 7$ (as the injectivity length of these states is $L = 3$).

3. *Characterization of the SLOCC classes*

From the results of the previous section we conclude that normal GHZ-generated states can be separated into three different sets according to their symmetries, where states from different sets are in different SLOCC classes:

1. $\chi(b) \neq -1, 0$ (case (ia) of Section V A 2): These states have only 1 nontrivial symmetry, which is global. We call this set the generic set as it contains almost all MPS.

2. $\chi(b) = -1$ (case (ib) of Section V A 2): These states have 2^N symmetries. This set contains the cluster state and thus we refer to it as the cluster set.

3. $\chi(b) = 0$ (case (iia) of Section V A 2): These states have only the trivial symmetry and thus we refer to this set as the symmetryless set.

In the following we determine the SLOCC classes within these sets. Using the symmetries (43) of the GHZ state and Corollary 1 of the main text this is straightforward and reveals the following SLOCC classification within the sets 1. to 3.:

1. First, we determine when $\Psi(GHZ_b)$ and $\Psi(GHZ_c)$ (with $\chi(b), \chi(c) \notin \{-1, 0\}$) are related via a (trivial) global operation. This is the case iff G_{GHZ} contains a $(b \to c)$-1-cycle. It is straightforward to show that this condition is satisfied iff $\chi(b) = \chi(c)$. Next, we have to determine the MPS that are related via $(b \to c)$-N-cycles with $N > 1$. To this end, we use the procedure explained in the paragraph after Corollary 1 in the main text. For two operators

$$h_1 = g_1 \otimes x_1 \otimes y_1^T \equiv s_{GHZ}^{(k,v_1,v_2)} \in G_{GHZ}, \tag{58}$$

$$h_2 = g_2 \otimes x_2 \otimes y_2^T \equiv s_{GHZ}^{(l,w_1,w_2)} \in G_{GHZ} \tag{59}$$

we define the matrix,

$$M \equiv y_1^{-1} y_2 \otimes (x_2^{-1} x_1)^T = (\sigma_1^k P_{v_2})^{-1} \sigma_1^l P_{w_2} \otimes \left[(\sigma_1^l P_{w_1})^{-1} \sigma_1^k P_{v_1} \right]^T. \tag{60}$$

As explained in the main text, h_1, h_2 form a $(b \to c)$-2-cycle iff there exists a $\lambda \neq 0$ such that

$$M\vec{b} = \lambda \vec{b}. \tag{61}$$

For any b that solves Eq. (61) we can find the corresponding c as

$$c = y_2 b x_1 = \sigma_1^l P_{w_2} b \sigma_1^i P_{v_1}, \tag{62}$$

as explained in the main text. In this way, we can show that $\Psi(GHZ_b), \Psi(GHZ_c)$ are related via a $(b \to c)$-2-cycle iff $\chi(b) = \frac{1}{\chi(c)}$. Analogously, we can show that $\Psi(GHZ_b), \Psi(GHZ_c)$ are not related via a $(b \to c)$-N-cycle of any size if neither $\chi(b) = \chi(c)$ nor $\chi(b) = \frac{1}{\chi(c)}$ hold. Summarizing, we have just shown the following,

$$GHZ_b \overset{N}{\sim} GHZ_c \;\Leftrightarrow \chi(b) = \begin{cases} \chi(c) \text{ or } \chi(c)^{-1} \text{ and } N \text{ even} \\ \chi(c) \text{ and } N \text{ odd.} \end{cases} \tag{63}$$

In particular, there are infinitely many, N-dependent SLOCC classes within this generic set.

Let us also briefly outline an alternative way to derive Eq. (63). For all fixed pairs of matrices b, c (with $\chi(b), \chi(c) \notin \{-1, 0\}$) one could explicitly determine all $h_1, h_2 \in G_A$ as in Eqs. (58 - 59) that are $(b \to c)$-connected. Note that

$$h_1 \xrightarrow{b \to c} h_2 \;\Leftrightarrow\; y_2 b x_2 \propto c \;\Leftrightarrow\; \sigma_1^k P_{y_2} \cdot b \cdot \sigma_1^l P_{z_1} \propto c. \tag{64}$$

For fixed b, c there are only very few or no h_1, h_2 that solve Eq. (64). For the b, c for which there are elements of G_A that can be $(b \to c)$-connected it is then straightforward to find all $(b \to c)$-N-cycles for $N = 1, 2$ and show that there are no larger cycles. This then leads to Eq. (63).

2. All MPS in this symmetry class are related to each other via (trivial) 1-cycles and are thus SLOCC equivalent for any N.

3. All MPS in this symmetry class are related to each other via (trivial) 1-cycles and are thus SLOCC equivalent for any N.

B. MPS generated by W-type states

1. *Characterization of the normal MPS*

Analogously to the GHZ case, we first have to determine when $\Psi(W_b)$ is normal. That is, we have to check for which $b \in GL(2, \mathbb{C})$ there is an L such that

$$\operatorname*{span}_{i_1, \ldots, i_L} \left\{ A_{W,b}^{i_1} \cdot \ldots \cdot A_{W,b}^{i_L} \right\} = \mathbb{C}^{2 \times 2}. \tag{65}$$

Here, we determine the minimal L with this property, i.e., the injectivity length of $\Psi(W_b)$. A straightforward calculation shows that the following cases have to be distinguished:

(i) $b_{ij} \neq 0$ for all i, j: $L = 2$ and thus $\Psi(W_b)$ is normal for $N \geq 5$.

(ii) exactly one entry of b is zero:

(iia) $b_{00} = 0$: $\Psi(W_b) \propto |0\rangle^{\otimes N}$ and, thus, these states are not normal.

(iib) else: $L = 2$ and thus $\Psi(W_b)$ is normal for $N \geq 5$.

(iii) exactly two entries of b are zero:

(iiia) $b_{01}, b_{10} = 0$: $L = 2$ and thus $\Psi(W_b)$ is normal for any $N \geq 5$.

(iiib) else: $\Psi(W_b)$ is a product state and therefore not normal.

2. *Characterization of the local symmetries*

The local symmetries of the W state are given by [10]

$$S_W = \left\{ \frac{1}{x} \begin{pmatrix} x & -y-z \\ 0 & \frac{1}{x} \end{pmatrix} \otimes \begin{pmatrix} x & y \\ 0 & \frac{1}{x} \end{pmatrix} \otimes \begin{pmatrix} x & z \\ 0 & \frac{1}{x} \end{pmatrix} \right\}_{(x,y,z)\in\mathbb{C}^{\times 3}}, \tag{66}$$

For the cases (i), (iib) and (iiia) of normal states determined in the last section, G_{W_b} contains the trivial cycle (from $\mathbb{1}$ to $\mathbb{1}$) and a continuous set of nontrivial 2-cycles. Hence, $\Psi(W_b)$ has only the trivial symmetry if N is odd and infinitely many symmetries if N is even. Interestingly, these symmetries have the same form for all W-generated normal MPS, namely

$$S_{\Psi(W_b)} = \begin{cases} \mathbb{1} & \text{if } N \text{ is odd,} \\ \left\{ \left(z(x) \otimes z(\frac{1}{x}) \right)^{\otimes \frac{N}{2}} \right\}_{x\in\mathbb{C}^\times} & \text{if } N \text{ is even,} \end{cases} \tag{67}$$

where

$$z(x) = \begin{pmatrix} x & (x - \frac{1}{x}) \frac{b_{01}+b_{10}}{b_{00}} \\ 0 & \frac{1}{x} \end{pmatrix}. \tag{68}$$

C. Characterization of the SLOCC classes

The order of the symmetries of normal W-generated states cannot be used to distinguish SLOCC classes. The reason for this is that all such states are SLOCC equivalent. To see this, we consider a normal MPS $\Psi(W_b)$ from case (iiia) in Section V B 1, i.e., with $b_{01} = b_{10} = 0$ and $b_{00}, b_{11} \neq 0$, and an arbitrary normal MPS $\Psi(W_c)$. Then G_A contains a $(b \to c)$-1-cycle for these choices of b, c. Hence, $\Psi(W_b) \overset{N}{\sim} \Psi(W_c)$ holds for any N and the normal states in (iiia) can be transformed to any other normal W-generated MPS via a (trival) global transformation. Consequently, all normal W-generated MPS are in the same SLOCC class.

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Chapter 4

Conclusion and Outlook

Our understanding of condensed matter systems is based on quantum mechanics. The exponential scaling of the Hilbert space with the number of particles, however, makes modeling many-body systems a daunting task. There are many ways to get around this curse of dimension, including Monte Carlo methods, variational ansatzes, quantum simulation and the investigation of exactly solvable models. Tensor Network States (TNS) provide us with such tools to gain insights into the behavior of condensed matter systems. First, it can be used as a variational ansatz, since it defines a set of states that can approximate ground states of relevant Hamiltonians using a small number of parameters. The extremely successful DMRG algorithm, for example, can be reformulated as a variational algorithm over MPS, and algorithms inspired by higher-dimensional TNS also have have gained popularity in recent years. Second, TNS provide us with tools to create and investigate exactly solvable models. The importance of these models is that both the ground and the low-energy excited states have extremely simple representations, thus helping to understand how certain complex phenomena emerge in these systems.

This Thesis was centered around the mathematical investigation of Tensor Networks. These investigations shed light onto the reasons why and how Tensor Networks are so successful in describing many-body systems. In the first part of the Thesis, we introduced TNS such as MPS, PEPS, MERA and TTN. We have given a review about the current state of the art of the theory of MPS and PEPS. We have shown first that all states can be written as TNS, but this description is not necessarily efficient. We have seen that if one only wants to approximate a state, then more efficient descriptions are possible. Apart from the possibility of representing states efficiently, the success of MPS is rooted in the fact that calculating expectation values of local observables with these states is extremely simple. This is not the case anymore with PEPS, which is partially the reason why algorithms based on them are less successful. The understanding of how these expectation values are calculated in MPS then naturally leads to a decomposition of TI MPS to a sum of smaller bond dimensional TI MPS. There is no known corresponding decomposition of PEPS. Another difference is that in MPS, renormalization fixed points are completely understood, whereas for PEPS, such a characterization is still missing, though through the bulk-boundary correspondence the characterization of RG fixed points of MPDO can

be thought of as one. A possible use of the framework of TN is the characterization of different phases (at least those that also have an RG fix point in them). We have shown how this is done in one dimensions in the case of SPT and also shown how topologically ordered phases can emerge in two dimensions.

In the second part of the thesis, I have included my publications. First, we have investigated how far PEPS can approximate certain states – a question necessary to understand if one is looking for a good variational ansatz. In Section 3.1 we have proven that PEPS can approximate thermal states of local Hamiltonians efficiently (the number of parameters needed for the approximation scales only polynomially with the system size), which is an improvement over the previously existing bounds. In Section 3.2 we have then provided a quantum algorithm for preparing Gibbs states and injective PEPS. For classical Hamiltonians, this results in an algorithm where we were able to prove an exponentially better run-time bound than the existing bounds for the corresponding classical Monte Carlo algorithm. In Section 3.3 we introduced a class of PEPS that encompasses the states for which the previous algorithm works. It also contains several other physically relevant states such as those used for the SPT classification in two dimensions. We have proven a fundamental theorem for this class of tensors, namely, under which circumstances such two tensors can generate the same states. This theorem leads to a better understanding of the SPT classification. In Section 3.4 we have used our understanding of MPS to characterize states that arise during the investigation of lattice gauge theories. We have shown how local symmetries can arise in these tensor networks. In Section 3.5 we generalized the fundamental theorem of injective PEPS to any normal non-translationally invariant MPS and PEPS. With this generalization one can readily investigate local symmetries as in Section 3.4, as well as arbitrary geometries such as higher-dimensional PEPS or states defined on hyperbolic lattices. In Section 3.6 we have then provided arguments that a general fundamental theorem is not expected to exist for PEPS. Instead, one has to restrict the input tensors for which such a theorem can work. Finally, in Section 3.7 we used the fundamental theorem from Section 3.5 to investigate of entanglement properties of MPS. This new fundamental theorem is required in order to deal with the not translationally invariant setting of entanglement theory.

Despite recent developments, there are several open questions concerning the structure of TNS, and in particular that of PEPS. For example, a well defined renormalization process is still missing for them. Such a definition would lead to the complete understanding of renormalization fixed points. There are also open questions concerning Fundamental Theorems of PEPS: deciding when two tensors generate the same state, in the most general case, is hopeless. It is therefore important to find new classes of tensors for which this question can be answered. Such classes might be G-injective or MPO-injective tensors. A Fundamental Theorem for these tensors then would lead to an SET classification. Finally, there are several other topics concerning the theory of TNS that we haven't mentioned. Such topics are, for example, the existence of continuum or infinite system size limits. I believe that understanding the structure of TNS will eventually also lead to better and more general algorithms.

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