Preparing projected entangled pair states on a quantum computer

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We present a quantum algorithm to prepare injective PEPS on a quantum computer, a problem raised by Verstraete, Wolf, Perez-Garcia, and Cirac [1]. To be efficient, our algorithm requires well-conditioned PEPS projectors and, essentially, an inverse-polynomial spectral gap of the PEPS' parent Hamiltonian. Injective PEPS are the unique groundstates of their parent Hamiltonians and capture groundstates of many physically relevant many-body Hamiltonians, such as e.g. the 2D AKLT state. Even more general is the class of G-injective PEPS which have parent Hamiltonians with a ground state space of degeneracy $|G|$, the order of the discrete symmetry group G. As our second result we show how to prepare G-injective PEPS under similar assumptions as well. The class of G-injective PEPS contains topologically ordered states, such as Kitaev's toric code which our algorithm is thus able to prepare.

Projected Entangled Pair States, or PEPS [2], have been proposed as a class of quantum states especially suited to describe the ground states of local Hamiltonians in quantum many-body physics. PEPS are a higher-dimensional generalization of the one-dimensional Matrix Product States [3], or MPS, for which many interesting properties have been proven: For example, MPS provably approximate the ground state of 1D local Hamiltonians with constant spectral gap [4, 5], exhibit an area law [5] as well as an exponential decay of two-point correlation functions. Furthermore, for each MPS with the *injectivity* property [6], a parent Hamiltonian can be constructed with this MPS as its unique ground state. MPS can also be prepared efficiently on a quantum computer [7]. PEPS however form a much richer class of states, and can e.g. represent critical systems and systems with topological quantum order [1]. It is conjectured that all ground states of gapped local Hamiltonians in higher dimensions can be represented faithfully as PEPS, and although there are strong indications for this fact, this has not been proven. What is clear, however, is the fact that one can also construct parent Hamiltonians for them [6], and the PEPS will be the unique ground states of those Hamiltonians if the PEPS obeys the so-called injectivity condition [6]. Many physically relevant classes of PEPS on lattices are known to be almost always injective, including e.g. the 2D AKLT state [6]. A particularly interesting subclass of PEPS is the one that consists of all those states whose parent Hamiltonian have a gap that scales at most as an inverse polynomial as a function of the system size: in that case, a local observable (i.e. the local Hamiltonian) allows to distinguish the state from all other ones, as the ground state always has energy zero by construction. Almost all PEPS that arise in a physical context supposedly fall into that class. It was an open problem whether such states could however be even created on a quantum computer, as an algorithm that would allow to prepare any PEPS would allow for the solution of PP-complete problems [8].

Our main result is to show that well-conditioned injective PEPS can be prepared on a quantum computer efficiently.

Theorem 1. *Let (V, E) be an interaction graph with bounded degree and some total order defined on V. Let $\{A^{(v)}\}_{v\in V_{[t]}}$ be a set of injective PEPS projectors associated with each v in V up to vertex t (according to the total vertex order) describing a sequence of PEPS $|\psi_t\rangle$, and let $\kappa = \max_{v\in V} \kappa(A^{(v)})$ be the largest condition number of all PEPS projectors. Let $\Delta = \min_t \Delta(H_t)$, where $\Delta(H_t)$ is the spectral gap of the parent Hamiltonian H_t of the PEPS $|\psi_t\rangle$. Then there exists a quantum algorithm generating the final PEPS $|\psi_{|V|}\rangle$ with probability at least $1-\varepsilon$ in time $O(|V|^2|E|^2\kappa^2\varepsilon^{-1}\Delta^{-1})$.*

The key idea of our approach is to grow the PEPS step by step. We demand that not only our final PEPS is the unique ground state of its parent local Hamiltonian, but also that there exists a sequence of partial sums of the local terms of the parent Hamiltonian, such that each partial sum has a unique ground state of its own. Based on this assumption, the algorithm starts with a physical realization of the valence bond pairs as its initial state and iteratively performs entangling measurements on the virtual particles to map virtual degrees of freedom to physical ones, just as in the definition of the PEPS. The PEPS is called injective, iff this map is (left) invertible which can only be the case if the dimension of the physical space is actually at least as large as the dimension of the virtual space at each vertex. Preparing a PEPS by measurements may seem to require post-selection to project onto the right measurement outcome. To overcome this issue we use the Marriott-Watrous trick [9, 10] of undoing a measurement based on Jordan's lemma [11] and combine it with the uniqueness property of injective PEPS [6] to prepare the required eigenstates. A key el-

ement that contributes to the success of this algorithm is the fact that the measurements are not done locally, such as in the framework of dissipative quantum state engineering [12], but globally by running a phase estimation algorithm that singles out the ground subspace; a similar approach was used in the context of the quantum Metropolis sampling algorithm [13]. The full paper describing the preparation of injective PEPS is available on the arXiv [17].

The creation of exotic quantum states is arguably one of the most challenging goals of current physics. While many interesting families of quantum states can be prepared by the above algorithm, the technical assumption of "injectivity" excludes the preparation of particularly intersting states with topological quantum order, since the injectivity property immediately excludes parent Hamiltonians with degenerate ground states. On the other hand, it is well known, that PEPS are in fact able to describe such phases of matter when one relaxes the injectivity condition and allows for a slightly more general class of states [14–16].

As our second result, we show that it is possible to generalize the previously stated result to this larger class of PEPS, with only minor modifications in the algorithm. One can relax the requirement of injectivity to a class of PEPS which are referred to as G-injective PEPS [18]. A G-injective PEPS is defined with respect to some finite symmetry group G that is acting on the virtual indices of the PEPS tensor. The requirement of G-injectivity reduces to two points: First, that the PEPS is invariant under the symmetry group G and second, that the PEPS tensor posesses a left inverse on the G-symmetric subspace. A central feature of the G-injective PEPS is that the parent Hamiltonian construction yields a Hamiltonian that has a degenerate ground state manifold. The degeneracy is given by the order of the group $|G|$, if the PEPS tensor is invariant under a semi-regular representation of the group, i.e a representation which contains a copy of each irrep of the group. The class of G-injective PEPS is therefore much richer and entails states that are known to possess topological order, such as topological spin liquids, states corresponding to Kitaev's quantum doubles and other quantum states that exhibit non-abelian topological order.

Even though preparing G-injective PEPS only requires a minor modification of the algorithm, the analysis proves more challenging, since at each step of the algorithm we construct a projector, by making use of the quantum phase estimation subroutine, which projects on the ground state manifold of the corresponding parent Hamiltonian. As already stated, in the case of G-injective PEPS this ground state is no longer unique. However, the assumption of uniqueness of the state was an important ingredient in the analysis of the algorithm for the injective PEPS. In fact, this problem can be overcome as long as the boundaries of the state are still open, by constructing appropriate boundary Hamiltonians to select one particular state from the degenerate ground state subspace. We are therefore only confronted with a degenerate ground state space during the final steps of the algorithm, when we start to close the boundaries. However, thanks to the PEPS structure, the crucial application of Jordan's lemma ([17, Lemma III.2]) generalises in this special case, and the degeneracy during the final stages of the algorithm does not change the performance significantly. We give the result in Theorem 2, which establishes almost the same runtime result for the G-injective case as Theorem 1 does for the simpler injective case, only with a modified effective condition number of the local tensors, the PEPS condition number κ_G, which is defined as follows:

Definition 1 (PEPS condition number)**.** *For a local G-injective PEPS tensor $A^{(v)}$ we define the the condition number as*

$$\kappa_v = \frac{\sigma_{\max}\left(A^{(v)}\big|_{S_G}\right)}{\sigma_{\min}\left(A^{(v)}\big|_{S_G}\right)}, \tag{1}$$

where S_G labels the symmetrtic subspace of the group G and $\sigma_i(A)$ denote the singular values of the map $A^v : \otimes^k \mathbb{C}^D \to \mathbb{C}^d$. The PEPS condition number κ_G for a PEPS (V, E) is then defined as $\kappa_G = \max_{v\in V} \kappa_v(A^{(v)})$.

This number can be understood as the maximal condition number, i.e. the ratio between the largest and the smallest singular value, of the PEPS map restricted to the invariant subspaces of the irreducible representations of the group G. If we restrict the map to the invariant subspaces, we are ensured that $\kappa_G < \infty$, because the assumption of G-injectivity ensures that the restrictions of the PEPS maps are invertible. With this quantity at hand the total runtime scaling of the algorithm can be expressed in the following theorem.

Theorem 2 ([19])**.** *Let (V, E) be an interaction graph with bounded degree and some total order defined on V. Let $\{A^{(v)}\}_{v\in V_{[t]}}$ be a set of G-injective PEPS projectors associated with each v in V up to vertex t (according to the total vertex order) describing a sequence of PEPS $|\psi_t\rangle$, and let κ_G be the PEPS condition number. Let $\Delta = \min_t \Delta(H_t)$, where $\Delta(H_t)$ is the spectral gap of the parent Hamiltonian H_t of the PEPS $|\psi_t\rangle$. Then there exists a quantum algorithm generating the final PEPS $|\psi_{|V|}\rangle$ with probability at least $1-\varepsilon$ in time $O(|V|^2|E|^2\kappa_G^2\varepsilon^{-1}\Delta^{-1})$.*

[1] F. Verstraete, M. Wolf, D. Perez-Garcia, and J. Cirac, Physical review letters **96**, 220601 (2006).

[2] F. Verstraete and J. Cirac, Physical Review A **70**,

60302(R) (2004), arXiv:quant-ph/0311130.
[3] S. Rommer and S. "Ostlund, Physical Review B **55**, 2164 (1997).
[4] F. Verstraete and J. Cirac, Physical Review B **73**, 94423 (2006).
[5] M. Hastings, Journal of Statistical Mechanics: Theory and Experiment **2007**, P08024 (2007).
[6] D. Perez-Garcia, F. Verstraete, J. I. Cirac, and M. M. Wolf, Quant. Inf. Comp **8**, 0650 (2008), arXiv:0707.2260.
[7] C. Schön, E. Solano, F. Verstraete, J. Cirac, and M. Wolf, Physical review letters **95**, 110503 (2005).
[8] N. Schuch, M. Wolf, F. Verstraete, and J. Cirac, Physical review letters **98**, 140506 (2007).
[9] C. Marriott and J. Watrous, Computational Complexity **14**, 122 (2005).
[10] D. Nagaj, P. Wocjan, and Y. Zhang, QIC **9**, 1053 (2009), arXiv:0904.1549.
[11] C. Jordan, Bull. Soc. Math. France **3**, 103 (1875).
[12] F. Verstraete, M. Wolf, and J. Cirac, Nature Physics **5**, 633 (2009), arXiv:0803.1447.
[13] K. Temme, T. Osborne, K. Vollbrecht, D. Poulin, and F. Verstraete, Nature **471**, 87 (2011).
[14] N. Schuch, D. Perez-Garcia, and I. Cirac, Arxiv preprint arXiv:1010.3732 (2010).
[15] O. Buerschaper, M. Aguado, and G. Vidal, Physical Review B **79**, 085119 (2009).
[16] X. Chen, B. Zeng, Z.-C. Gu, I. L. Chuang, and X.-G. Wen, Phys. Rev. B **82**, 165119 (2010).
[17] M. Schwarz, K. Temme, and F. Verstraete, (2011), arXiv:1104.1410.
[18] N. Schuch, I. Cirac, and D. Pérez-García, Annals of Physics **325**, 2153 (2010).
[19] T. Cubitt, D.-P. Garcia, M. Schwarz, K. Temme, and F. Verstraete, "Constructing G-injective PEPS on a quantum computer," (2011), unpublished.