A TENSOR VERSION OF THE QUANTUM WIELANDT THEOREM[*]

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Abstract. We prove boundedness results for the injectivity regions for projected entangled pair states. Our result is a higher-dimensional generalization of the quantum Wielandt inequality.

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1. Introduction. In [8], Sanz et al. proved a quantum version of the Wielandt inequality. This theorem was motivated by the study of matrix product states (MPS) and conjectures stated in [5]. We refer the reader to [1, section 1] for an introduction to mathematical quantum physics in general and MPS in particular. In summary, in quantum physics the data corresponding to a system is described by a vector in a Hilbert space, or tensor products of these spaces. Physical observables are described by linear Hermitian operators on these spaces where the eigenvalues of those operators correspond to the possible values of the observable and the eigenspaces to the possible states of the system after an observation is done. The operator for the energy of a system is called the Hamiltonian and of particular interest are the eigenstates corresponding to the lowest eigenvalues, also called ground states. MPS provide an efficient description of eigenstates of local gapped Hamiltonians.

The local Hamiltonian of which a given MPS is a ground state is called the parent Hamiltonian of the MPS. The quantum Wielandt theorem proved upper bounds on the support of parent Hamiltonians for injective MPS, which was the final piece missing for proving that the manifold of MPS is in one to one correspondence with ground states of local gapped Hamiltonians [2].

In mathematical terms, the quantum Wielandt theorem can be stated as follows. Let $\mathcal{A} = (A_1, \ldots, A_d)$ be a d-tuple of $D \times D$-matrices, and assume that there is an N such that the linear span of $\{A_{i_1} \cdots A_{i_N} | 1 \leq i_j \leq d\}$ equals the space of $D \times D$-matrices. Then already for $N = C(D, d) := (D^2 - d + 1)D^2$, the linear span of $\{A_{i_1} \cdots A_{i_N} | 1 \leq i_j \leq d\}$ equals the space of $D \times D$-matrices. The bound $C(D, d)$ was recently improved to $O(D^2 \log D)$ in [4] and is conjectured to be $O(D^2)$ [5].

The two-dimensional generalizations of MPS are called projected entangled pair states (PEPS) and play a central role in the classification of the different quantum phases of spin systems defined on two-dimensional grids. PEPS are much more

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complex than MPS: just as MPS can be understood in terms of completely positive maps on matrices, PEPS deal with completely positive maps on tensors, for which no analogues of eigenvalue and singular value decompositions exist. It has been a long-standing open question in the field of quantum tensor networks whether an analogue of the quantum Wielandt theorem exists for PEPS, which is the missing piece in proving that every PEPS has a parent Hamiltonian with finite support—cf. [1, section 2] and references therein. This paper proves the existence of such a theorem, albeit in a weaker form than for MPS as the upper bound is nonconstructive. In physics terms, it is proven that the notion of injectivity for PEPS is well defined, in the sense that there is only a finite amount of blocking needed for the map from the virtual to the physical indices to become injective.

The bounds for quantum Wielandt theorem in [8, 4, 7] were obtained using explicit methods from linear algebra. Our main new insight is the application of nonconstructive Noetherian arguments from nonlinear algebra. For MPS, our theorem is equivalent to Conjecture 1 in [5].

2. PEPS and injective regions. By a *grid* we mean a triple $G = (\mathcal{V}, E_I, E_O)$, where $\mathcal{V}, E_I, E_O$ are finite sets, respectively called vertices, inner edges, and outgoing edges. We will write $E = E_I \cup E_O$. One can think of a grid as (a part of) a system of particles, where the vertices are the particles and the edges indicate interaction between the particles. Every inner edge e may be identified with a two-element subset $\{v_1, v_2\}$ of $\mathcal{V}$. Every outgoing edge distinguishes one element of $\mathcal{V}$, which we call its endpoint. For v a vertex, $e(v)$ will denote the set of edges incident with that vertex. Let G be a grid. To every edge e of G we associate a finite-dimensional $\mathbb{C}$-vector space V_e, equipped with a perfect pairing $V_e \otimes V_e \to \mathbb{C}$. To every vertex v of G, we associate two $\mathbb{C}$-vector spaces: the *virtual space* $V_v := \bigotimes_{e \in e(v)} V_e$ and the *physical space* W_v, which represents the physical state of the particle.

Let $(v \mapsto A_v)_{v \in G}$ be a function that assigns to every vertex v of G a tensor $A_v \in V_v$. Then we have

$$\bigotimes_{v \in \mathcal{V}} A_v \in \bigotimes_{v \in \mathcal{V}} V_v \cong \bigotimes_{e \in E_O} V_e \otimes \bigotimes_{e \in E_I} V_e^{\otimes 2}.$$

Using the pairing $V_e^{\otimes 2} \to \mathbb{C}$, we obtain a new tensor in $\bigotimes_{e \in E_O} V_e$. This tensor will be denoted by $\mathcal{C}[(v \mapsto A_v)_{v \in G}]$, or simply by $\mathcal{C}[v \mapsto A_v]$. Graphically, operation $\mathcal{C}$ is represented by contracting all inner edges in the grid.

Example 2.1 (multiplication of matrices). Let G be the following grid:

$$\text{—}\square\text{—}\square\text{—}$$
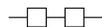
with vertices 1 and 2. Then $\mathcal{C}[(v \mapsto A_v)_{v \in G}]$ is simply the matrix product $A_1 A_2$.

Typically, grids without outgoing edges are used to represent tensors in $\bigotimes_{v \in \mathcal{V}} W_v$. This is done as follows. One fixes for every vertex v an element ϕ_v in $V_v \otimes W_v$. There are several ways one can think about ϕ_v:

- If we extend the grid with an additional outgoing edge e_v at every vertex, and associate to it the space W_v, we may identify ϕ_v with A_v from the previous paragraph.
- By identifying V_v with its dual, we may identify ϕ_v with a map $V_v \to W_v$.
- As a subspace of V_v, by contracting with W_v, i.e., the image of $W_v \to V_v$.

By the first point, we obtain a tensor $\mathcal{C}[(v \mapsto \phi_v)_{v \in G}]$ in $\bigotimes_{e \in E_O} V_e \otimes \bigotimes_{v \in \mathcal{V}} W_v$. In particular, if our original grid has no outgoing edges, this corresponds to a physical

state of our system, i.e., an element of $\bigotimes_{v \in \mathcal{V}} W_v$. Any state that arises in this way is called a *PEPS*.

We now give a description in coordinates. Write $d_v = \dim W_v$, $D_e = \dim V_e$, and suppose ϕ_v is given by

$$\sum_{i=1}^{d_v} \sum_{\boldsymbol{j}} A_{i,\boldsymbol{j}}^{(v)} |i, \boldsymbol{j}\rangle,$$

where the second sum is over all tuples $\boldsymbol{j} = (j_e)_{e \in e(v)}$, $1 \le j_e \le D_e$. Then

$$\mathcal{C}[v \mapsto \phi_v] = \sum_{i_1, i_2, \dots = 1}^{d} \mathcal{C}[v \mapsto A_{i_v}^{(v)}] \otimes |i_1, i_2, \dots\rangle \in \bigotimes_{e \in E_O} V_e \otimes \bigotimes_{v \in \mathcal{V}} W_v.$$

DEFINITION 2.2. *The tensor $\mathcal{C}[v \mapsto \phi_v]$ may be identified with a map $\bigotimes_{e \in E_O} V_e \to \bigotimes_{v \in \mathcal{V}} W_v$. If this map is injective, we say that $(G, \{\phi_v\}_{v \in \mathcal{V}})$ is an injective region. Equivalently, $(G, \{\phi_v\}_{v \in \mathcal{V}})$ is an injective region if and only if the tensors $\mathcal{C}[v \mapsto A_{i_v}^{(v)}]$ span the whole space $\bigotimes_{e \in E_O} V_e$.*

3. Main theorem. We fix natural numbers n (grid dimension), D (bond dimension), and d (physical dimension). For $N_1, \dots, N_n \in \mathbb{N}$, we let $G = G(N_1, \dots, N_n)$ be the n-dimensional square grid of size $N_1 \times \cdots \times N_n$. In particular, every vertex has degree $2n$. The grid $G(3, 5)$ is presented below:
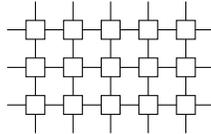
We will denote the outgoing edges of G by $(\boldsymbol{j}, \pm \mathbf{e}_i)$, where $\boldsymbol{j}$ is a vertex on the boundary of the grid, and $\pm \mathbf{e}_i$ indicates the direction of the outgoing edge.

To every edge e we associate the vector space $V_e = V = \mathbb{C}^D$. We stress that D is now the same for every edge. Now we can identify all virtual spaces $V_v = \bigotimes_{e \in e(v)} V_e = (\mathbb{C}^D)^{\otimes \deg(v)} = (\mathbb{C}^D)^{\otimes 2n}$ in the obvious way: the tensor factor of $(\mathbb{C}^D)^{\otimes \deg(v)}$ associated to an edge out of v will be identified with the tensor factor of $(\mathbb{C}^D)^{\otimes \deg(w)}$ associated to the edge out of w pointing in the same direction. We also identify all physical spaces W_v with a fixed d-dimensional vector space.

Having done these identifications, we can now associate to every vertex the same $\phi_{\mathcal{A}} = \sum_{i=1}^{d} \sum_{\boldsymbol{j}} A_{i,\boldsymbol{j}} |i, \boldsymbol{j}\rangle$, where $\mathcal{A} = (A_1, \dots, A_d)$ is a collection of d tensors $A_i \in (\mathbb{C}^D)^{\otimes 2n}$. From now on, we will assume we have a fixed $\mathcal{A}$ and let the size of the grid $G = G(N_1, \dots, N_n)$ vary.

DEFINITION 3.1. *We say that G is an injective region for $\mathcal{A}$ if $(G, \{\phi_{\mathcal{A}}\}_{v \in \mathcal{V}})$ is an injective region. Explicitly, G is an injective region for $\mathcal{A}$, if the tensors $\mathcal{C}[(v \mapsto A_{i_v})_{v \in G}]$ linearly span whole space $(\mathbb{C}^D)^{\otimes E_O(G)}$, when we consider all possible ways of placing a tensor from $\mathcal{A}$ at every vertex of G. If $\mathcal{A}$ has an injective region, we say that $\mathcal{A}$ is injective.*

Remark 3.2. We note that being an injective region for G and being injective are properties of the linear span of $\mathcal{A}$, not a particular choice of tensors A_i.

In the following lemma we prove that being an injective region is stable under extension of the grid.

LEMMA 3.3. *Let $G_1 \subseteq G_2$ be n-dimensional square grids. If G_1 is an injective region for $\mathcal{A}$, then so is G_2.*

Proof. By induction, we may assume that $G_1 = G(N_1 - 1, N_2, \ldots, N_n)$ and $G_2 = G(N_1, N_2, \ldots, N_n)$. If $N_1 = 2$ the statement is true, because G_2 is the union of two injective regions; cf. [6, Lemma 1]. Thus we assume $N_1 > 2$. The vertices of G_2 will be identified with vectors $\boldsymbol{j} = (j_1, \ldots, j_n) \in \mathbb{N}^n$ with $1 \leq j_i \leq N_i$. Such a vertex is in G_1 if additionally $j_1 \leq N_1 - 1$. We need to show that every tensor $T \in V^{\otimes E_O(G_2)}$ can be written as a linear combination of tensors of the form $\mathcal{C}[(\boldsymbol{j} \mapsto A_{i_j})_{\boldsymbol{j} \in G_2}]$. In fact it is enough to show this for rank one tensors T, since every tensor is a linear combination of rank one tensors.

We can identify $E_O(G_1)$ with a subset of $E_O(G_2)$ as follows. To an outgoing edge $(\boldsymbol{j}, \pm \mathbf{e}_i)$ of $E_O(G_1)$, we associate $(\boldsymbol{j}, \pm \mathbf{e}_i)$ if $\pm \mathbf{e}_i \neq +\mathbf{e}_1$ and $(\boldsymbol{j} + \mathbf{e}_1, +\mathbf{e}_1)$ if $\pm \mathbf{e}_i = +\mathbf{e}_1$. Assuming T has rank one, we have $T = T_1 \otimes T_2 \in V^{\otimes E_O(G_1)} \otimes V^{\otimes r}$, where r equals the cardinality of $E_O(G(N_2, \ldots, N_n))$.
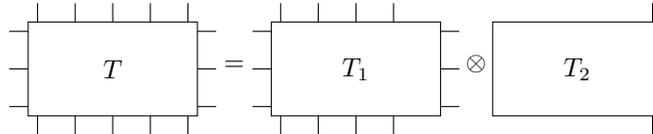

By assumption we can write T_1 as a linear combination of tensors of the form $\mathcal{C}[(\boldsymbol{j} \mapsto A_{i_j})_{\boldsymbol{j} \in G_1}]$. Let G_1' be the grid obtained from G_1 by contracting all inner edges among vertices $\boldsymbol{j}$ for which $j_1 > 1$. This grid is the rightmost one in the picture below. In particular, all vertices with $j_1 > 1$ get identified to a vertex v_1. Then T_1 is in particular a linear combination of tensors of the form $\mathcal{C}[(v \mapsto B_v)_{v \in G_1'}]$, where $B_v = A_{i_v}$ if v is one of the vertices that did not get contracted and $B_{v_1} = \mathcal{C}[(\boldsymbol{j} \mapsto A_{i_j})_{\boldsymbol{j} \in G_1, j_1 > 1}]$.
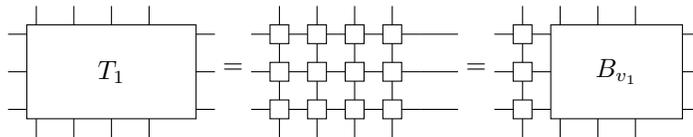
Consider the tensors $B_{v_1} \otimes T_2 \in V^{\otimes |E_O(G_1)|}$. By assumption each one is a linear combination of tensors of the form $\mathcal{C}[(\boldsymbol{j} \mapsto A_{k_j})_{\boldsymbol{j} \in G_1}]$, where now we identified G_1 with the subgrid of G_2 consisting of all vertices $\boldsymbol{j}$ with $j_1 > 1$.

Thus, we see that T is a combination $\mathcal{C}[(\boldsymbol{j} \mapsto A_{s_j})_{\boldsymbol{j} \in G_2}]$ where s may be identified with i above for $\boldsymbol{j}$ such that $j_1 = 1$ and with k when $j_1 > 1$.
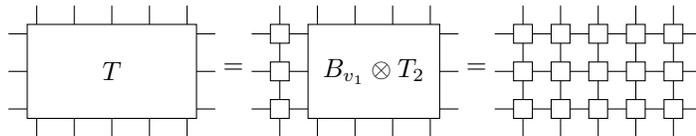
Our main theorem says that if $\mathcal{A}$ is injective, then there exists an injective region of bounded size (where the bound only depends on our parameters D, d, n). More precisely, we have the following.

THEOREM 3.4. *Let $G_1 \subset G_2 \subset \cdots \subset G_k \subset \cdots$ be a chain of n-dimensional grids. Then there exists a constant C (depending on D, d, and the chain) such that the following holds:*

> If $\mathcal{A} \in (\mathbb{C}^D)^{\otimes 2n} \otimes \mathbb{C}^d$ is chosen so that for some k, G_k is an injective region for $\mathcal{A}$, then already G_C is an injective region for $\mathcal{A}$.

Proof. For any grid G and $\mathcal{A} \in ((\mathbb{C}^D)^{\otimes 2n})^d$, we write $S_G(\mathcal{A}) := \{\mathcal{C}[(v \mapsto A_{i_v})_{v \in G}]\}$ $\subseteq (\mathbb{C}^D)^{\otimes E_O(G)}$, and $V_G := \{\mathcal{A} \in ((\mathbb{C}^D)^{\otimes 2n})^d | \operatorname{Span}(S_G(\mathcal{A})) \subsetneq (\mathbb{C}^D)^{\otimes E_O(G)}\}$. Thus, G is an injective region for $\mathcal{A}$ if and only if $\operatorname{Span}(S_G(\mathcal{A})) = (\mathbb{C}^D)^{\otimes E_O(G)}$ if and only if $\mathcal{A} \notin V_G$.

By Lemma 3.3, it holds that $V_{G_1} \supseteq V_{G_2} \supseteq \cdots \supseteq V_{G_k} \supseteq \cdots$. We need to show that this chain eventually stabilizes. We will show that every V_{G_k} is a Zariski closed subset of $((\mathbb{C}^D)^{\otimes 2n})^d$, i.e., that is the zero locus of a system of polynomials. This will finish the proof by Hilbert basis theorem.

Fix a grid $G = G_k$. For every $\mathcal{A} \in ((\mathbb{C}^D)^{\otimes 2n})^d$, we can build a $D^{E_O(G)} \times d^{|\mathcal{V}(G)|}$ matrix $M_{\mathcal{A}}$ whose entries are the coefficients of the elements of $S_G(\mathcal{A})$. The condition $\operatorname{Span}(S_G(\mathcal{A})) \subsetneq (\mathbb{C}^D)^{\otimes E_O(G)}$ is equivalent to $M_{\mathcal{A}}$ having rank smaller than $D^{E_O(G)}$. The entries of $M_{\mathcal{A}}$ are polynomials in the entries of $\mathcal{A}$. Hence, the condition $\mathcal{A} \in V_G$ can be expressed as the vanishing of certain polynomials ($D^{E_O(G)}$-minors of $M_{\mathcal{A}}$) in the entries of $\mathcal{A}$. Hence, V_G is a Zariski closed subset of $((\mathbb{C}^D)^{\otimes 2n})^d$. $\square$

Theorem 3.4 can be reformulated as follows.

THEOREM 3.5. *There exists a finite collection of grids $G_1, \ldots, G_M$ (depending on n, D, d) such that the following holds:*

> *If $\mathcal{A} \in ((\mathbb{C}^D)^{\otimes 2n})^d$ is injective, then one of the G_i is an injective region for $\mathcal{A}$.*

The equivalence of Theorems 3.4 and 3.5 follows from the following general lemma.

LEMMA 3.6. *Let $\mathcal{P}$ be a partially ordered set. We consider $\mathbb{N}^n$ with the coordinatewise partial order. Let $f : \mathbb{N}^n \to \mathcal{P}$ be a map such that*
  1. *$\boldsymbol{a}_1 \leq \boldsymbol{a}_2 \implies f(\boldsymbol{a}_1) \geq f(\boldsymbol{a}_2)$,*
  2. *for every chain $\boldsymbol{a}_1 < \boldsymbol{a}_2 < \ldots$ in $\mathbb{N}^n$, the chain $f(\boldsymbol{a}_1) \geq f(\boldsymbol{a}_2) \geq \ldots$ stabilizes after finitely many steps.*
Then there is a finite subset B of $\mathbb{N}^n$ such that for any $\boldsymbol{a} \in \mathbb{N}^n$, there is a $\boldsymbol{b} \in B$ with $\boldsymbol{a} \geq \boldsymbol{b}$ and $f(\boldsymbol{a}) = f(\boldsymbol{b})$.

Proof. We first claim that there is a $\boldsymbol{b}_0 \in \mathbb{N}^n$ such that $f(\boldsymbol{a}) = f(\boldsymbol{b}_0)$ for every $\boldsymbol{a} \geq \boldsymbol{b}_0$. Indeed, if there was no such $\boldsymbol{b}_0$ we could build an infinite chain $\boldsymbol{a}_1 < \boldsymbol{a}_2 < \ldots$ in $\mathbb{N}^n$ with $f(\boldsymbol{a}_1) > f(\boldsymbol{a}_2) > \ldots$.

Now we can proceed by induction on n: the subset $\{\boldsymbol{a} \in \mathbb{N}^n | \boldsymbol{a} \not\geq \boldsymbol{b}_0\}$ can be written as a finite union of hyperplanes, each of which can be identified with $\mathbb{N}^{n-1}$. By the induction hypothesis, in each such hyperplane $H \subset \mathbb{N}^n$ there is a finite subset $B_H \subset H$ such that for any $\boldsymbol{a} \in H$, there is a $\boldsymbol{b} \in B_H$ with $\boldsymbol{a} \geq \boldsymbol{b}$ and $f(\boldsymbol{a}) = f(\boldsymbol{b})$. We define B as b_0 together with the union of all B_H. $\square$

Proof of Theorem 3.5. We apply Lemma 3.6 by identifying $\mathbb{N}^n$ with the collection of n-dimensional grids and taking $\mathcal{P}$ to be the poset of subsets of $((\mathbb{C}^D)^{\otimes 2n})^d$ ordered by inclusion, and $f : G \mapsto V_G$, where V_G was defined in the proof of Theorem 3.4. We conclude by Theorem 3.4. $\square$

Remark 3.7. In the case $n = 1$, Theorem 3.5 is equivalent to the existence of a bound on the length of products of matrices that generate the whole space of matrices. This is known as the *quantum Wielandt theorem*; see [5, Conjecture 1]. An effective version was proved in [8, 4].

We note that the constants in Theorems 3.4 and 3.5 can be chosen independent of d.

COROLLARY 3.8. *For any n and D there exists a finite collection of grids $G_1, \ldots,$ G_M such that the following holds:*

> *For any d, if $\mathcal{A} \in ((\mathbb{C}^D)^{\otimes 2n})^d$ is injective, then one of the G_i is an injective region for $\mathcal{A}$.*

Proof. By Remark 3.2 it is enough to consider the subspaces $\langle \mathcal{A} \rangle \subset ((\mathbb{C}^D)^{\otimes 2n})$. In particular the dimension of the subspaces is bounded by D^{2n} and for each fixed dimension we obtain a finite number of grids by Theorem 3.5. $\square$

Further we have the following computational implication.

COROLLARY 3.9. *For every fixed n and D, there exists an algorithm to decide if $\mathcal{A}$ is injective.*

Proof. Let $G_1, \ldots, G_M$ be the set of grids from Corollary 3.8. The algorithm checks for every i whether G_i is an injective region for $\mathcal{A}$. For a fixed grid, this amounts to checking surjectivity of a given polynomial map; cf. [3]. We know $\mathcal{A}$ is injective if and only if it is injective for one of the G_i. $\square$

We note that although we know such an algorithm exists, we cannot explicitly provide it. The reason is that we do not know the grids $G_1, \ldots, G_M$ from Corollary 3.8—we just know they exist. Our result should also be contrasted with [9, Theorem 4], which states that there is no algorithm that receives ϕ_v and decides if $\mathcal{C}[(v \mapsto \phi_v)_{v \in T_{x,y}}] = 0 \ \forall x, y \in \mathbb{N}$, where $T_{x,y}$ is the $x \times y$-torus.

REFERENCES

[1] J. I. CIRAC, J. GARRE-RUBIO, AND D. PÉREZ-GARCÍA, *Mathematical Open Problems in Projected Entangled Pair States*, preprint, arXiv:1903.09439, 2019.

[2] M. FANNES, B. NACHTERGAELE, AND R. F. WERNER, *Finitely correlated states on quantum spin chains*, Comm. Math. Phys., 144 (1992), pp. 443–490.

[3] C. HARRIS, M. MICHAŁEK, AND E. C. SERTÖZ, *Computing images of polynomial maps*, Adv. Comput. Math. (2019), pp. 1–21, https://doi.org/10.1007/s10444-019-09715-8.

[4] M. MICHAŁEK AND Y. SHITOV, *Quantum version of Wielandt's inequality revisited*, IEEE Trans. Inform. Theory, 65 (2019), pp. 5239–5242, https://doi.org/10.1109/TIT.2019.2897772.

[5] D. PEREZ-GARCIA, F. VERSTRAETE, M. M. WOLF, AND J. I. CIRAC, *Matrix product state representations*, Quantum Info. Comput., 7 (2007), pp. 401–430.

[6] D. PÉREZ-GARCIA, F. VERSTRAETE, M. M. WOLF, AND J. I. CIRAC, *PEPS as unique ground states of local hamiltonians*, Quantum Info. Comput., 8 (2007).

[7] M. RAHAMAN, *A New Bound on Quantum Wielandt Inequality*, preprint, arXiv:1807.06872, 2018.

[8] M. SANZ, D. PEREZ-GARCIA, M. M. WOLF, AND J. I. CIRAC, *A quantum version of Wielandt's inequality*, IEEE Trans. Inform. Theory, 56 (2010), pp. 4668–4673.

[9] G. SCARPA, A. MOLNAR, Y. GE, J. J. GARCIA-RIPOLL, N. SCHUCH, D. PEREZ-GARCIA, AND S. IBLISDIR, *Computational Complexity of PEPS Zero Testing*, preprint, arXiv:1802.08214, 2018.