

Rigorous Rg Algorithms and Area Laws for Low Energy Eigenstates In 1D

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Abstract

One of the central challenges in the study of quantum many-body systems is the complexity of simulating them on a classical computer. A recent advance [8] gave a polynomial time algorithm to compute a succinct classical description for unique ground states of gapped 1D quantum systems. Despite this progress many questions remained unresolved, including whether there exist rigorous efficient algorithms when the ground space is degenerate (and $\text{poly}(n)$ dimensional), or for the $\text{poly}(n)$ lowest energy states for 1D systems, or even whether such states admit succinct classical descriptions or area laws.

In this paper we give a new algorithm for finding low energy states for 1D systems, based on a rigorously justified renormalization group (RG)-type transformation. In the process we resolve some of the aforementioned open questions, including giving a polynomial time algorithm for $\text{poly}(n)$ degenerate ground spaces and an $n^{O(\log n)}$ algorithm for the $\text{poly}(n)$ lowest energy states for 1D systems (under a mild density condition). We note that for these classes of systems the existence of a succinct classical description and area laws were not rigorously proved before this work. The algorithms are natural and efficient, and for the case of finding unique ground states for frustration-free Hamiltonians the running time is $\tilde{O}(nM(n))$, where $M(n)$ is the time required to multiply two $n \times n$ matrices.

1998 ACM Subject Classification F.2.1 Numerical Algorithms and Problems, J.2 Physical Sciences and Engineering

Keywords and phrases Hamiltonian complexity, area law, gapped ground states, algorithm

Digital Object Identifier 10.4230/LIPIcs.ITCS.2017.46

* I. Arad's research was partially performed at the Centre for Quantum Technologies, funded by the Singapore Ministry of Education and the National Research Foundation, also through the Tier 3 Grant random numbers from quantum processes.

† The author acknowledges support by ARO Grant W911NF-12-1-0541, NSF Grant CCF-1410022 and Templeton Foundation Grant 52536.

‡ The author acknowledges support by ARO Grant W911NF-12-1-0541, NSF Grant CCF-1410022 and Templeton Foundation Grant 52536.

§ T. Vidick was partially supported by the IQIM, an NSF Physics FrontiersCenter (NSF Grant PHY-1125565) with support of the Gordon and Betty Moore Foundation (GBMF-12500028).



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8th Innovations in Theoretical Computer Science Conference (ITCS 2017).

Editor: Christos H. Papadimitrou; Article No. 46; pp. 46:1–46:14

Leibniz International Proceedings in Informatics



LIPICs Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

1 Introduction

One of the central challenges in the study of quantum many-body systems is the classical complexity of finding low energy states of local Hamiltonians. This problem is the quantum analog of constraint satisfaction problems, and is known to be QMA-complete, even for one-dimensional Hamiltonians [1]. This means that we do not even expect that there is a sub-exponential size classical description of the ground state that allows efficient computation of local observables such as the energy. In sharp contrast, the widely used heuristic density matrix renormalization group (DMRG) algorithm invented two decades ago [14] has been remarkably successful in practice on one-dimensional (1D) problems. A recent advance [8] resolved this seeming contradiction by giving a polynomial time algorithm to actually compute a succinct classical description for unique ground states of quantum systems coming from *gapped* 1D Hamiltonians.

In this paper we give a fundamentally different algorithm that applies to a significantly larger class of 1D Hamiltonians, namely:

1. *Hamiltonians with a degenerate gapped ground space:* H has smallest eigenvalue ε_0 with associated eigenspace of dimension $r = \text{poly}(n)$, and second smallest eigenvalue ε_1 such that $\varepsilon_1 - \varepsilon_0 \geq \gamma$.
2. *Gapless Hamiltonians with a low density of low-energy states:* The dimension of the space of all eigenvectors of H with eigenvalue in the range $[\varepsilon_0, \varepsilon_0 + \eta]$, for some constant $\eta > 0$, is $r = \text{poly}(n)$.

For both classes of Hamiltonians, our results show the existence of succinct representations in the form of matrix product states (MPS) for a basis for (a good approximation to) the ground space (resp. low energy subspace) of the Hamiltonian. The bond dimension of the MPS is polynomial in r and n and exponential in μ^{-1} (respectively η^{-1} in case 2). Furthermore the algorithms return these MPS descriptions in polynomial time for the first case and quasi-polynomial time in the second. For the special case of finding unique ground states for frustration-free Hamiltonians the algorithm is particularly efficient, with a running time of $\tilde{O}(nM(n))$, where $M(n)$ is the time required to multiply two $n \times n$ matrices.

Our results should be understood in the context of a substantial body of prior work studying ground state entanglement in 1D systems. Central to this work is the so-called *area law for entanglement entropy* — a conjecture which states that in ground states of gapped local Hamiltonians the entanglement entropy of a region scales as its surface area, rather than its volume. A landmark result by Hastings [5] proved this conjecture for gapped 1D systems with unique ground state, and a sequence of follow up results substantially strengthened the bounds (see, for example, the review article Ref. [4]). However, the techniques for these results break down for low energy and degenerate ground states, and few results were known for these questions: Chubb and Flammia [3] extended the approach from Ref. [8] and subsequent improvements from Ref. [6] to establish an efficient algorithm (and area law) for gapped Hamiltonians with a constant degeneracy in the ground space. Masanes [9] proves an area law with logarithmic correction under a strong assumption on the density of states, together with an additional assumption on the exponential decay of correlations in the ground state.

Our algorithm hinges on novel ideas that can be viewed as giving a rigorous underpinning to the well known Renormalization Group (RG) formalism within condensed matter physics [15]. This formalism occupies a central place in many-body physics and provides a sweeping computational approach to the “physically relevant corner of Hilbert space” by suggesting that such states can be coarse-grained at different levels of granularity, or length scales,

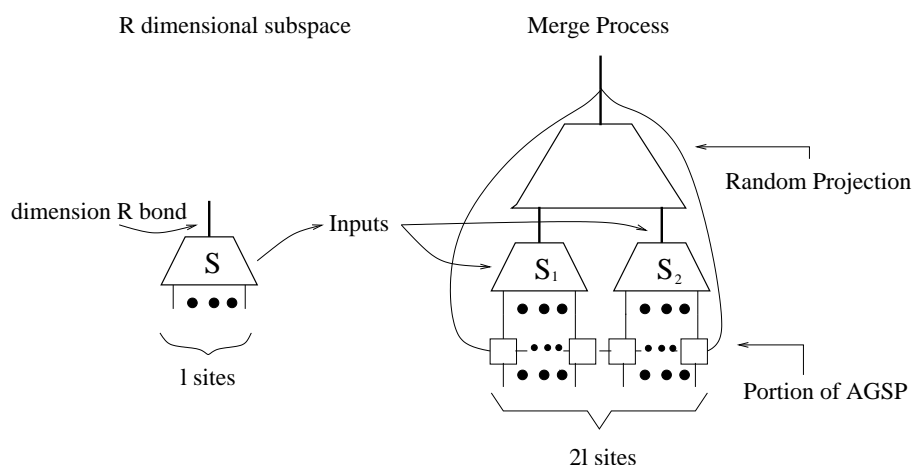
thereby iteratively eliminating the irrelevant degrees of freedom. There are recent suggestions that RG may be intimately related to feature extraction and the success of deep nets [10].

The new algorithm relies on three innovations. The first innovation starts with the idea that if our goal is to approximate a subspace T (of low energy states, say) on n qubits, the algorithm can make progress by locally maintaining a small dimensional subspace S on k particles, with the property that T is close to $S \otimes X$ where X is the entire Hilbert space on the remaining $n - k$ particles. A major challenge here is measuring the quality of this partial solution. This is accomplished by a suitable generalization of the definition of a viable set introduced in [8] to the setting of a target subspace T , and is one of the conceptual contributions of this paper.

As the number of qubits k on which the partial solution lies is increased, the fundamental challenge is to keep the dimension of the subspace S , which will otherwise naturally grow exponentially, polynomial, while maintaining the quality of the solution which will otherwise decay. To address this, we design a two step process: we deal with the dimension problem by projecting onto a small random subspace. Of course this degrades the quality i.e. blows up the error. So in turn, we control the error by the application of an AGSP, an operator with small entanglement rank which preserves low-energy states while reducing the norm of high energy states. The success of this two-step process depends upon the construction of a suitable class of AGSPs — uniform AGSPs — that ensures a favorable tradeoff between dimension and error between random projection and AGSP. The two-step process may be visualized as a (two stroke) pump: the first step (random projection) reduces the dimension, but leaves the dimension-error tradeoff essentially unchanged. The second step (AGSP) improves the dimension-error tradeoff sufficiently, so that the two steps together restore both dimension and error to their values at the start of the iteration.

The third innovation is to design an algorithm whose analysis does not rely on an area law: instead of processing one particle per iteration, it acts in parallel on all sites at each iteration, merging the results along a binary tree. Consequently, the algorithm uses only $O(\log(n))$ iterations. This is important because besides the number of quantum states stored (the dimension of the subspace S), the running time of the algorithm is also governed by the description complexity (bond dimension) of these states. The bond dimension grows exponentially with the number of iterations, yielding an $n^{O(\log n)}$ algorithm.

A tensor network picture of the resulting process, called Merge, is provided in the figure below.¹ Beginning with inputs representing subspaces of ℓ qubits shown on the left, the Merge process (shown on the right) outputs a representation of a small subspace on 2ℓ qubits.



¹ We are grateful to Christopher T. Chubb for originally suggesting these pictures to us.

The algorithm iteratively applies the Merge process. The overall construction results in a partial isometry that is reminiscent of a MERA [12, 13], and it should be fruitful to compare and contrast them as well as to standard RG. In particular, both our construction and RG build subspaces in a binary tree fashion. However, whereas RG can be realized as a tensor network on a binary tree (where each node represents the partial isometry associated with selecting only a small portion of the previous space), the use of the AGSP in our construction allows for selection of the small subspace outside the tensor product of the previous two spaces.

This hierarchical merge process establishes a new operational description of the entanglement structure of the low energy states of local Hamiltonians in 1D. It allows us to prove an area law for poly(n) degenerate ground spaces and (up to log correction) for low energy states, and is the basis of the rigorously justified RG transformation.

Our new algorithms could potentially be made very efficient. The main bottlenecks are the complexity of the AGSP and the MPS bond dimension that must be maintained. In the case of a frustration-free Hamiltonian with unique ground state we obtain a running time of $O(2^{O(1/\gamma^2)} n^{1+o(1)} M(n))$, where $M(n)$ is matrix multiplication time. This has an exponentially better scaling in terms of the spectral gap γ (due to avoidance of the ε -net argument) and saves a factor of $n/\log n$ (due to the logarithmic, instead of linear, number of iterations) as compared to an algorithm for the same problem considered in [6]. We speculate that it might further be possible to limit the bond dimension of all MPS considered to $n^{o(1)}$ (instead of $n^{1+o(1)}$ currently), which, if true, would imply a nearly-linear time $O(n^{1+o(1)})$ algorithm.

Organization of the paper

We start with some preliminaries and notation in Section 2. Section 3 introduces our main tool, the Merge process, and employs it to derive an area law for 1D gapped Hamiltonian with polynomial degeneracy in the ground space. In Section 4 we build on the approach to develop an efficient algorithm for the same systems. The constructions of AGSP that underlie our results, as well as the algorithm for the case of gapless Hamiltonians with a low density of low-energy states, are described in the full version of this paper [2].

2 Preliminaries and Notation

We begin by describing the basic setup for our results.

► **Definition 1.** Let $H = \sum_{i=1}^n h_i$ be a local Hamiltonian acting on the Hilbert space

$$\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^d \otimes \dots \otimes \mathbb{C}^d \simeq (\mathbb{C}^d)^{\otimes n}$$

associated with a 1D chain of n qudits, each of local dimension d . Each h_i is assumed to be a non-negative operator with norm at most 1 acting on the i -th and $(i+1)$ -st qudits. We denote by $\varepsilon_0 \geq 0$ the smallest eigenvalue (ground energy) of H , and consider the following assumptions:

- (FF) **Frustration-Free:** H is frustration-free ($\varepsilon_0 = 0$) with a unique ground state $|\Gamma\rangle$ and a spectral gap $\gamma > 0$ above the ground state. In this case we let $T = \text{Span}\{|\Gamma\rangle\}$ denote the one-dimensional ground space of H .
- (DG) **Degenerate Gapped:** H has a degenerate ground space T of dimension $r = \text{poly}(n)$, along with a spectral gap $\gamma > 0$ above the ground space.

For $A \subseteq \{1, \dots, n\}$ we denote the Hilbert associated with the qudits in A by \mathcal{H}_A , e.g. $\mathcal{H}_{[1,3]} = \mathbb{C}^d \otimes \mathbb{C}^d \otimes \mathbb{C}^d$ corresponds to the first three qudits. Separately, for any operator (Hamiltonian) H , $H_{[a,b]}$ will denote the subspace spanned by the eigenvectors of H with eigenvalues in the interval $[a, b]$. For a set S of vectors we denote by P_S the orthogonal projection onto the span of S and refer to $\dim(\text{Span}(S))$ as the *size* of S , denoted $|S|$. We often identify sets of vectors with the vector space they span.

We use standard $O(\cdot)$, $o(\cdot)$, $\Omega(\cdot)$, $\omega(\cdot)$ and $\Theta(\cdot)$ notation. The use of a tilde, such as $\tilde{O}(\cdot)$, will indicate a polylogarithmic overhead, i.e. $\tilde{O}(f) = O(f \text{ poly log } f)$. We use $f = \text{poly}(n)$ to mean that there is a fixed polynomial p such that $f(n) \leq p(n)$ for all n .

3 Viable sets, the merge process, and area laws

Recall that our goal is to formalize and analyze an RG-like transformation in the spirit of the following claim, which for ease of explanation we state for the gapped degenerate case:

► **Proposition 2.** *Let H be a local Hamiltonian satisfying Assumption (DG) (q.v. Definition 1).*

1. *For every length scale ℓ and contiguous block A of ℓ qudits, there is a subspace $S \subseteq \mathcal{H}_A$ of dimension $q = r^{1+o(1)} e^{\tilde{O}(\frac{1}{r} \log^3 d)}$ such that S approximates the ground space T of H , in the following sense: every state in T has large overlap with a state whose reduced density matrix on \mathcal{H}_A is supported on S .*
2. *Suppose given two subspaces $S_1 \subseteq \mathcal{H}_1$ and $S_2 \subseteq \mathcal{H}_2$ on adjacent blocks of ℓ qudits each, such that each of S_1, S_2 has dimension at most q and approximates T . Then it is possible to generate a subspace $S \subseteq \mathcal{H}_1 \otimes \mathcal{H}_2$ of the composite system that has the same dimension q and approximates T to the same extent as S_1, S_2 .*

The key feature of the second item in the proposition is that the dimension of the merged set S has not increased: the set has the same size as S_1, S_2 separately, and yet it combines all the information each of these sets holds about the restriction of the ground space T to \mathcal{H}_1 and \mathcal{H}_2 respectively.

As we will see, the first item in the proposition leads naturally to an area law and succinct MPS representations for good approximations to states in T . The proof of the first item will be obtained by iteratively performing the merging procedure described in the second item. With additional work the merging procedure can be made efficient, leading to an efficient algorithm for computing these succinct representations.

3.1 Viable sets

We formalize the notion of a subspace *approximating* another as follows.

► **Definition 3.** A subspace T is δ -close to a subspace T' if

$$P_{T'} P_T P_{T'} \geq (1 - \delta) P_{T'}.$$

We say that T and T' are *mutually δ -close* if each is δ -close to the other, and denote by $\angle_m(T, T')$ the smallest δ such that T, T' are mutually δ -close.

Geometrically,

$$\angle_m(T, T') = 1 - \min_{\substack{x \in T \\ \|x\|=1}} \max_{\substack{x' \in T' \\ \|x'\|=1}} |x \cdot x'|^2$$

is the squared sine of the largest principal angle between the subspaces T and T' (where the cosines of the principal angles are given by the singular values of $P_T P_{T'}$); in particular the statement that T is δ -close to T' is equivalent to the fact that for every $|\psi\rangle \in T'$ there exists $|\phi\rangle \in T$ such that $|\langle\psi|\phi\rangle|^2 \geq 1 - \delta$. Note that mutually close subspaces always have the same dimension.

With a view towards working with subsystems, we extend the notion of closeness to capture approximation by subspaces defined only on one half of a factored Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$.

► **Definition 4.** Given a subspace $T \subseteq \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, a subspace $S \subseteq \mathcal{H}_A$ is δ -viable for T if

$$P_T P_{S_{ext}} P_T \geq (1 - \delta) P_T, \quad (1)$$

where $S_{ext} := S \otimes \mathcal{H}_B$.

This definition generalizes the definition of a viable set from Ref. [8], which was specialized to the case where T is a one-dimensional subspace containing a unique ground state. Informally it captures the notion that a reasonable approximation of T can be made using the subspace $S \otimes \mathcal{H}_B$. With the definition in place, we can make the statement of item 1 of Proposition 2 precise. For ease of exposition we relax the dependence of q on r to $\tilde{O}(r^2)$.

► **Theorem 5.** *Let H be a local Hamiltonian satisfying Assumption (DG). Then for any block $A \subseteq \{1, \dots, n\}$ of $\ell \leq n$ qudits there exists a .015-viable set $S \subset \mathcal{H}_A$ for the ground space T of H of dimension at most $q = \tilde{O}(r^2) e^{\tilde{O}(\frac{1}{7} \log^3 d)}$.*

We further note that the dependence of q on the dimension r can be improved to $\tilde{O}(r)$, using a direct “bootstrapping” argument that is slightly different from the more “algorithmic” argument that we give in Section 3.3. This improved bound and bootstrapping argument are presented in the full version [2].

While the notion of viable set is quite intuitive for small δ , our arguments will also involve viable sets with parameter δ close to 1, a regime where there is less intuition. A helpful interpretation of the definition is that it formalizes the fact that for a viable set S , the image of the unit ball of S_{ext} when projected to T contains the ball of radius $(1 - \delta)$.

► **Lemma 6.** *If S is δ -viable for T then for every $|t\rangle \in T$ of unit norm, there exists an $|s\rangle \in S_{ext}$ such that $P_T |s\rangle = |t\rangle$ and $\| |s\rangle \| \leq \frac{1}{1-\delta}$.*

The proof of this and the following two useful lemmas appear in the full version [2]. The first summarizes the effect of tensoring two viable sets supported on disjoint spaces.

► **Lemma 7.** *Suppose S_1, S_2 are δ_1 -viable and δ_2 -viable for T respectively, defined on disjoint sets of qudits. Then the set $S := S_1 \otimes S_2$ is $(\delta_1 + \delta_2)$ -viable for T .*

The second lemma shows that our notion of closeness can be chained together and is compatible with the notion of viable set:

► **Lemma 8.** *If T is δ -close to T' and T' is δ' -close to T'' then T is $2(\delta + \delta')$ -close to T'' . Consequently if S is δ -viable for T and T is δ' -close to T' then S is $2(\delta + \delta')$ -viable for T' .*

3.2 The Merge Process

We are ready to outline the merging procedure referred to in item 2 of Proposition 2, which lies at the heart of our RG transformation. Assume we are given a decomposition $\mathcal{H} = \mathcal{H}_L \otimes (\mathcal{H}_1 \otimes \mathcal{H}_2) \otimes \mathcal{H}_R$ of the global Hilbert space. The merge process **Merge** takes as input two subsets $V_1 \subseteq \mathcal{H}_1$ and $V_2 \subseteq \mathcal{H}_2$ and returns a subset $V \subseteq \mathcal{H}_1 \otimes \mathcal{H}_2$. To do so, it requires two additional inputs: a finite set of operators $\{A_i\}_{i=1}^{D^2}$ each acting on $\mathcal{H}_1 \otimes \mathcal{H}_2$, along with a positive integer s . The procedure consists of the following three simple steps.

Merge($V_1, V_2, \{A_i\}, s$):

Step 1: Tensoring. Set $W = V_1 \otimes V_2$.

Step 2: Random Sampling. Let $W' \subseteq W$ be a random s -dimensional subspace of W .

Step 3: Error Reduction. Set $V = \text{Span}(\cup_i A_i W')$.

Return V.

The effectiveness of **Merge** relies on the properties of the operators $\{A_i\}$, with a sufficiently good choice of these operators leading to a formalization of item 2. of Proposition 2. Suitable operators can be obtained from the decomposition of an *approximate ground state projection* (AGSP). The detailed construction is given in the full paper [2]; the following theorem summarizes the essential properties of the resulting $\{A_i\}$.

► **Theorem 9** (Existence of AGSP, (DG)). *Let H be a local Hamiltonian satisfying Assumption (DG), and $\mathcal{H} = \mathcal{H}_L \otimes \mathcal{H}_M \otimes \mathcal{H}_R$ a decomposition of the n -qudit space in three contiguous blocks. There exists a collection of D^2 operators $\{A_i\}_{i=1}^{D^2}$ acting on \mathcal{H}_M along with a subspace $\tilde{T} \subseteq \mathcal{H}$ such that:*

- $\angle_m(T, \tilde{T}) \leq .005$,
- $D = e^{\tilde{O}(\frac{1}{\gamma} \log^3 d)}$,
- *There is $\Delta > 0$ such that $D^{12}\Delta \leq \frac{1}{2000}$ and whenever $S \subseteq \mathcal{H}_M$ is δ -viable for \tilde{T} then $S' = \text{Span}\{\cup_i A_i S\}$ is δ' -viable for \tilde{T} , with $\delta' = \frac{\Delta}{(1-\delta)^2}$.*

Given a finite collection of operators $\{A_i\}$ we denote by $\{A_i\}^k$ the set of all products of k of the A_i . The following theorem states the guarantees offered by the **Merge** process when initialized with operators $\{A_i\}$ satisfying the guarantees of Theorem 9.

► **Theorem 10.** *Let H be a local Hamiltonian satisfying Assumption (DG), and $\mathcal{H} = \mathcal{H}_L \otimes (\mathcal{H}_1 \otimes \mathcal{H}_2) \otimes \mathcal{H}_R$ a decomposition of the n -qudit space into contiguous blocks. Let $\{A_i\}$ and D be as in Theorem 9,*

$$s \geq 1600r(\log r + 1) \quad \text{and} \quad k = \frac{1}{2} \lceil \log_D(s) \rceil.$$

Let $V_1 \subseteq \mathcal{H}_1$ and $V_2 \subseteq \mathcal{H}_2$ be .015-viable subspaces for T of size $q = s^2$ each. Then with probability $1 - e^{-\Omega(s)}$ the space $V = \text{Merge}(V_1, V_2, \{A_i\}^k, s)$ is .015-viable for T with $|V| \leq q$.

The proof below analyzes the effect of each of the three steps of the **Merge** process. The first creates the trivial subspace $V_1 \otimes V_2$, whose dimension $q^2 = \dim(V_1) \dim(V_2)$ is too large, and whose overlap with T is worse than desired by a factor of 2. The random sampling step roughly evenly trades off size for overlap: it picks a random s dimensional subspace for $s \ll q$, at the expense of making the overlap roughly $\frac{s}{q^2}$. Finally, the application of the AGSP (via the operators $\{A_i\}$) blows up the size from s to at most q , while increasing overlap to at least the original overlap of V_1 and V_2 . This relies on the highly favorable D, Δ -tradeoff of the AGSP.

Proof. We analyze each of the three steps of the **Merge** process:

1. *Tensoring.* Applying Lemma 7 yields that the result of step 1, $W = V_1 \otimes V_2 \subseteq \mathcal{H}_1 \otimes \mathcal{H}_2$, is a .03 viable set for T of size q^2 . Using the first condition from Theorem 9 and applying Lemma 8, W is .07-viable for \tilde{T} .

2. *Random Sampling.* We show that at the end of this step, with high probability W' is $(1 - \alpha)$ -viable for \tilde{T} with $\alpha = (.8)s/q^2$. We accomplish this by establishing that with high probability $\|P_{W'_{ext}}|v\rangle\|^2 \geq \alpha$ for all states $|v\rangle \in \tilde{T}$, where $W'_{ext} = \mathcal{H}_L \otimes W' \otimes \mathcal{H}_R$ and $W_{ext} = \mathcal{H}_L \otimes W \otimes \mathcal{H}_R$.

Let $|v\rangle \in \tilde{T}$ have norm 1, and $|w\rangle = P_{W_{ext}}|v\rangle \in W_{ext}$. Using that W is .07-viable for \tilde{T} it follows that $\| |w\rangle \|^2 \geq .995$. Since $W'_{ext} \subseteq W_{ext}$, $P_{W'_{ext}}|v\rangle = P_{W'_{ext}}|w\rangle$. Applying a standard concentration argument it holds that $\|P_{W'_{ext}}|v\rangle\|^2 \geq (.9)(.995)^{\frac{s}{q^2}}$ with probability at least $1 - q^2 e^{-s/400}$.

By a simple volume argument (see e.g. [11, Lemma 5.2]) there exists a ν -net for the Euclidean unit ball of \tilde{T} consisting of at most $(1 + \frac{2}{\nu})^r$ elements of \tilde{T} , where $\nu = \sqrt{(.1)(.9)(.995)^{\frac{s}{q^2}}}$. Applying the preceding argument to each $|v\rangle$ in the net, a choice of s such that

$$\eta = \left(1 + \frac{2}{\nu}\right)^r q^2 e^{-s/400} < 1 \quad (2)$$

will guarantee that with probability at least $1 - \eta$, $\|P_{W'_{ext}}|v\rangle\|^2 \geq (.9)(.995)^{\frac{s}{q^2}}$ for all $|v\rangle$ in the net; hence $\|P_{W'_{ext}}|v\rangle\|^2 \geq (.99)(.9)(.995)^{\frac{s}{q^2}} \geq .8^{\frac{s}{q^2}}$ for all $|v\rangle \in \tilde{T}$ of unit norm. The equation (2) is satisfied with

$$s > 400 \left(2 \log q + \frac{r}{2} \log \left(1 + \sqrt{47 \frac{q^2}{s}} \right) \right),$$

a condition verified by the choices of s and q made in the theorem.

Step 3: Error Reduction. Applying Theorem 9 k times in sequence, $V = \text{Span}\{\{A_i\}^k \cdot W'\}$ is $\frac{\Delta^k}{(1-\delta)^2} = \frac{\Delta^k}{\alpha^2}$ -viable for T' of size at most $D^{2k}s$. Our choice of k ensures $D^{2k}s = q$, and the relation between D and Δ implies that

$$\frac{\Delta^k}{\alpha^2} = \frac{s^6 \Delta^k}{.64} = \frac{D^{12k} \Delta^k}{.64} \leq \frac{1}{(.64)} \frac{1}{2000} \leq .001.$$

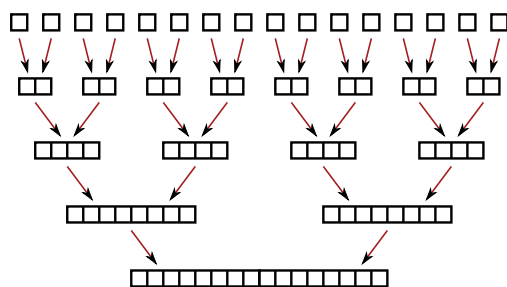
Thus V is .001-viable for \tilde{T} , and by Lemma 8 it is .012 < .015-viable for T . ◀

3.3 Area law for degenerate Hamiltonians

In this section we first prove Theorem 5 establishing the claim made in the first item of Proposition 2. From the theorem we then deduce an area law for local Hamiltonians satisfying Assumption (DG) (degenerate ground space with a spectral gap; q.v. Definition 1).

Proof of Theorem 5. Consider a system A of $\ell \leq n$ consecutive qudits; for ease of notation we'll assume that ℓ is a power of 2 and A consists of the first ℓ qudits of the n -qudit chain on which H acts. The proof of the theorem is based on the following iterative procedure for constructing the .015-viable set claimed in the theorem. The procedure depends on a set of operators $\{A_i\}$ obtained from Theorem 9 for various decompositions of \mathcal{H} , and we let s and k be as in the theorem.

The proof of Theorem 5 follows by showing that with positive probability Procedure 1 returns a subspace $V_1^{\log \ell}$ that is .015-viable for T and such that $|V_1^{\log \ell}| = \tilde{O}(r^2) e^{\tilde{O}(\frac{1}{\gamma} \log^3 d)}$.



■ **Figure 1** The parallel structure of Procedure 1. Each square represents a qudit, and successive viable sets are supported on neighboring groups of squares.

Procedure 1: Given a local Hamiltonian H satisfying(DG), returns a viable set for T supported on the first ℓ qudits.

Initialization: Set $V_j^0 = \mathcal{H}_j$ for $j = 1, 2, \dots, \ell$.

Iteration:

For $i = 1, \dots, \log(\ell)$ do:

For all $j \in \{1, 2, \dots, \frac{\ell}{2^i}\}$, set

$$V_j^i = \mathbf{Merge}(V_{2j-1}^{i-1}, V_{2j}^{i-1}, \{A_i\}^k, s) \subseteq \mathcal{H}_{[(j-1)2^i+1, j2^i]},$$

where $\{A_i\}$ are as in Theorem 9 for the decomposition

$$\mathcal{H} = \mathcal{H}_{[1, (j-1)2^i]} \otimes (\mathcal{H}_{[(j-1)2^i+1, (2j-1)2^{i-1}]} \otimes \mathcal{H}_{[(2j-1)2^{i-1}+1, j2^i]}) \otimes \mathcal{H}_{[j2^i+1, \ell]},$$

and s and k are as in Theorem 10.

Let $q = D^{2k}s$ be the size of the space output by **Merge**, and observe that by Theorem 9 it holds that $q = \tilde{O}(r^2)e^{\tilde{O}(\frac{1}{\gamma} \log^3 d)}$. We prove the result by induction, showing that V_j^i is .015-viable for T with $|V_j^i| \leq q$ for each i, j . The initialization step establishes this for $i = 0$ since each V_j^0 is 0-viable for T with $|V_j^0| = d$. The induction step is a direct consequence of Theorem 10, which establishes that at each iteration with probability $1 - e^{-\Omega(s)}$ the set $V_j^i = \mathbf{Merge}(V_{2j-1}^{i-1}, V_{2j}^{i-1}, s, \{A_i\}^k)$ is .015-viable for T with $|V_j^i| \leq q$. Each merging operation succeeds with independent probability, therefore there is a positive probability that the procedure terminates with a .015-viable set $V_1^{\log \ell}$ for T . ◀

An area law for gapped Hamiltonians with a degenerate ground space follows readily from Theorem 5. Indeed, for any desired cut Theorem 5 establishes the existence of 0.015-viable sets of size at most q for the block of qudits on either side of the cut. As a consequence each element of the ground space T has a constant approximation by a state of Schmidt rank at most q . Applying a suitable AGSP to the tensor product of two such viable sets one can obtain a δ -viable set, for any desired δ , at a modest (depending on δ) increase in size. This kind of trade-off leads to a standard proof bounding both the Schmidt rank and the von Neumann entropy across the cut for any state in the ground space. We state the result here, referring to the full version [2] for the proof.

► **Corollary 11** (Area law for degenerate gapped Hamiltonians). *Let H be a local Hamiltonian satisfying Assumption (DG). For any cut and any $\delta = \text{poly}^{-1}(n)$ there is subspace $S \subseteq \mathcal{H}$*

that is δ -close to T and such that every element of S has Schmidt Rank no larger than

$$s(\delta) = \tilde{O}(r^2) e^{\tilde{O}\left(\frac{1}{\gamma} \log^3 d\right)} \cdot e^{\tilde{O}\left(\gamma^{-1/4} \log^{3/4}\left(\frac{1}{\delta}\right) \log d\right)}.$$

Moreover, every state $|\psi\rangle \in T$ has entanglement entropy

$$S(|\psi\rangle\langle\psi|) \leq 4 \log r + \tilde{O}\left(\frac{1}{\gamma} \log^3 d\right)$$

and can be approximated by a state $|\psi'\rangle$ such that $|\langle\psi|\psi'\rangle| > 1 - \delta$ and $|\psi'\rangle$ has an MPS representation with bond dimension bounded by

$$\tilde{O}(r^2) e^{\tilde{O}\left(\frac{1}{\gamma} \log^3 d\right)} e^{\tilde{O}\left(\gamma^{-1/4} \log^{3/4}\left(\frac{1}{\delta}\right) \log d\right)}.$$

We note that the dependence on r in the bounds for the Schmidt rank and the bond dimension of the MPS approximation can be improved from $\tilde{O}(r^2)$ to $r^{1+o(1)}$. In fact there is a simpler way of getting these bounds through a clean “bootstrapping” argument, for which we refer to the full version [2].

4 Moving to algorithms

There are two main obstacles to turning Procedure 1 into an efficient algorithm. The first consists in showing that operators $\{A_i\}$ satisfying the conditions of Theorem 9 can be generated efficiently from a description of the Hamiltonian, and that it is possible to apply these operators efficiently, as required to complete the error reduction step of the **Merge** process. The following theorem states that this can be achieved.

► **Theorem 12** (Efficient AGSP, (DG)). *There exists a procedure **Generate**(H, M, ε'_M) which takes as input*

- A local Hamiltonian H satisfying Assumption (DG),
- A decomposition $\mathcal{H} = \mathcal{H}_L \otimes \mathcal{H}_M \otimes \mathcal{H}_R$ of the n -qudit space into contiguous blocks,
- An estimate ε'_M for the minimal energy ε_M of the restriction of H to \mathcal{H}_M such that $|\varepsilon_M - \varepsilon'_M| \leq 10$,

and returns

- MPO representations for a collection of D^2 operators $\{A_i\}_{i=1}^{D^2}$ acting on \mathcal{H}_M and of bond dimension at most $n^{\tilde{O}(\gamma^{-2})}$ satisfying the conditions of Theorem 9 for some subspace \tilde{T} ,
- An MPO for an operator \tilde{H}_M such that $\|\tilde{H}_M\| = O(\gamma^{-1} \log \gamma^{-1})$ and the minimal energy $\tilde{\varepsilon}_M$ of \tilde{H}_M restricted to \tilde{T} satisfies $|\varepsilon_M - \tilde{\varepsilon}_M| < 1/2$.

Moreover, **Generate**(H, M, ε'_M) runs in time $n^{\tilde{O}(\gamma^{-2})}$.²

The proof of Theorem 12 relies on new constructions of approximate ground state projections (AGSP), details of which are given in the full version [2]. The theorem guarantees that the $\{A_i\}$ can be constructed efficiently *provided* it is possible to provide a good approximation to the ground state energy of the restriction of H to \mathcal{H}_M . This is the reason for including \tilde{H}_M as parts of the output of **Generate**, which is then used by an additional step of *energy estimation* incorporated in Algorithm 2.

² Here and in all our estimates on running times we suppress dependence on the local dimension d , which is treated as a constant.

Algorithm 2: Given a local Hamiltonian H satisfying Assumption (GS), returns a set $V_1^{\log n}$ that is 0.015-close to the ground space T of H .

Initialization: Set $V_j^0 = \mathcal{H}_j$ and $\varepsilon'_{0,j} = 0$ for $j \in \{1, 2, \dots, n\}$.

Iteration:

For $i = 1, \dots, \log(n)$ and $j \in \{1 \dots \frac{n}{2^i}\}$ do:

Generate. Let $M = \{(j-1)2^i, (j-1)2^i + 1, \dots, j2^i - 1\}$, $\varepsilon'_M = \varepsilon'_{i-1, 2j-1} + \varepsilon'_{i-1, 2j}$.

Set $(\{A_i\}, \tilde{H}_M) = \mathbf{Generate}(H, M, \varepsilon'_M)$.

Merge. Set $V_j^i = \mathbf{Merge}'(V_{2j-1}^{i-1}, V_{2j}^{i-1}, \{A_i\}, s, k, \xi) \subseteq \mathcal{H}_{[(j-1)2^i+1, j2^i]}$, where s and k are specified in Theorem 10 and $\xi = \text{poly}^{-1}(n, r)$ is chosen small enough (see proof of Theorem 13).

New Energy Estimation. Form the subspace $V = \{A_i\}^t \cdot (V_{2j-1}^{i-1} \otimes V_{2j}^{i-1})$ for $t = \Theta(\log \gamma^{-1})$. Compute the smallest eigenvalue $\varepsilon'_{i,j}$ of the restriction of \tilde{H}_M to V .

Final step: Return $V_1^{\log n}$.

The second difficulty encountered in turning Procedure 1 into an algorithm is that, even if the $\{A_i\}$ can be applied efficiently, due to the logarithmic number of iterations it may be that the bond dimension of MPS representations for the elements of the viable sets we work with increase to super-polynomial. This difficulty can be overcome by introducing a *bond trimming* component Trim_ξ to the **Merge** procedure, resulting in the following modified procedure **Merge'** taking an additional trimming parameter ξ as input (ξ will usually be of order $\text{poly}^{-1}(n)$):

Merge'($V_1, V_2, \{A_i\}, s, k, \xi$):

Step 1: Tensoring. Set $W = V_1 \otimes V_2$.

Step 2: Random Sampling. Let $W' \subseteq W$ be a random s -dimensional subspace of W .

Step 3: Error Reduction. Set $V = W'$. Repeat k times:

Set $V = \text{Trim}_\xi(\text{Span}(\cup_i A_i V))$.

Return V .

Correctness of **Merge'** (for an appropriate choice of ξ) is based on the area law proven in Corollary 11. The details of the trimming³ procedure Trim_ξ , together with the analysis of **Merge'**, are given in the full paper [2].

The following theorem proves the correctness of Algorithm 2.

► **Theorem 13.** *Let H be a local Hamiltonian satisfying Assumption (DG). Then with probability at least $1 - \frac{1}{n}$ the set $V_1^{\log n}$ returned by Algorithm 2 is 0.015-viable for T .⁴ The running time of the algorithm is $n^{\tilde{O}(\gamma^{-2})}$.*

Proof. The proof mirrors the analysis of Procedure 1 given in the proof of Theorem 5 in Section 3.3; the two main differences are that we must show that at every step, with high enough probability the call to **Merge'** yields a good viable set and the **New Energy Estimation** step yields a sufficiently accurate energy estimate for the next iteration.

³ We note that the trimming procedure differs from that of [8]

⁴ The probability of success can be improved to $1 - \text{poly}^{-1}(n)$ by scaling the parameter s used in the algorithm by an appropriate constant.

Both conditions are satisfied at initialization since each V_j^0 is 0-viable for T with $|V_j^0| = d$ and the energy estimates are accurate since there are no terms of the Hamiltonian when restricting to single particles.

Assume V_{2j-1}^{i-1} and V_{2j}^{i-1} are both .015-viable for T with $|V_{2j-1}^{i-1}|, |V_{2j}^{i-1}| \leq q$, and $\varepsilon'_{i-1,2j-1}, \varepsilon'_{i-1,2j}$ both within an additive ± 3 of their respective true values (the ground state energy of the restriction of H to the corresponding spaces). As a result ε'_M is within 7 of the correct value ε_M , and by Theorem 12 **Generate** yields a set $\{A_i\}$ with the properties stated in Theorem 9. Thus by Theorem 10 V_j^i is .015-viable for T with probability $1 - e^{-\Omega(s)} \geq 1 - \frac{1}{n^2}$ (provided $r \geq \log n$, which we may always assume without loss of generality). For this we need to check Theorem 10 still applies when **Merge** is replaced by **Merge'**. The analysis of the trimming procedure given in [2] shows that this is the case provided the error reduction parameter Δ associated with the $\{A_i\}$ is replaced by $(\Delta + 2\sqrt{krs\xi})$; choosing $\xi = \text{poly}^{-1}(n, r)$ we may ensure that $2\sqrt{krs\xi} < .0001D^{-12}$. With this choice, the remaining calculation of 10 applies to still yields that V_j^i is .015-viable for T .

Once this has been established, an application of the third item from Theorem 9 shows that provided the constant implicit in the definition of t is chosen large enough the subspace V obtained after the **New Energy Estimation** step is $O(\gamma^2)$ -viable for \tilde{T} . Using that $\|\tilde{H}_M\| = O(\gamma^{-1} \log \gamma^{-1})$ it follows that $\varepsilon'_{i,j}$ is within an arbitrarily small constant of the minimal energy of \tilde{H}_M restricted to \tilde{T} . Using the last guarantee from Theorem 12, $\varepsilon'_{i,j}$ is within $\frac{3}{2}$ of the minimal energy ε_M of the restriction of H to \mathcal{H}_M . This completes the inductive step.

We have shown that the iterative step succeeds with probability at least $1 - 1/n^2$; since there are a total of n such merging steps, applying a union bound the final set $V_1^{\log n}$ is .015-viable with probability at least $1 - \frac{1}{n}$.

In total the complete algorithm requires only a polynomial number of operations on MPS representations of vectors. Due to trimming, all these vectors have polynomial bond dimension and thus each operation can be implemented in polynomial time. The complexity is dominated by the complexity of the procedure **Generate** and the application of the operators A_i , which is $n^{\tilde{O}(\gamma^{-2})}$. ◀

We end this section by noting that in case one desires a better than constant approximation to T the final step of Algorithm 2 can be replaced by the following:

Final step. Set $K = (\mathbb{1} - H/\|H\|)$ and $\tau = 10\|H\|\gamma^{-1} \log(1/\delta)$. Choose an orthonormal basis $\{|y_i^{(0)}\rangle\}$ for $V_1^{\log n}$. Repeat for $t = 1, \dots, \tau$:

$$\text{Set } \{|y_i^{(t)}\rangle\} = \text{Trim}_\xi(\text{Span}\{K|y_i^{(t-1)}\rangle\}).$$

Return $\{|z_i\rangle\}$, the smallest r eigenvectors of H restricted to $W = \text{Span}\{|y_i^{(\tau)}\rangle\}$.

The result of this step is a basis $\{|z_i\rangle\}$ for a subspace S such that $\angle_m(S, T) \leq \delta$.

Frustration-free Hamiltonians with a unique ground state

The computation-intensive step of the AGSP-based RG transformation introduced in Section 3 is the construction and subsequent application of the set of operators $\{A_i\}$. In the special case where the Hamiltonian H satisfies Assumption (FF), i.e. H is frustration-free and has a spectral gap, the operators $\{A_i\}$ can be constructed very efficiently, yielding strong bounds on the running time. We state a specialized theorem for this setting. The proof is given in the full version [2].

Algorithm 3: Given a local Hamiltonian H satisfying Assumption (FF), returns a δ -approximation to its ground state $|\Gamma\rangle$.

Initialization: Set $V_j^0 = \mathcal{H}_j$ for $j \in \{1, 2, \dots, n\}$.

Iteration:

For $i = 1, \dots, \log(n)$ and all $j \in \{1, \dots, \frac{n}{2^i}\}$,

Generate. Let $M = \{(j-1)2^i, (j-1)2^i + 1, \dots, j2^i - 1\}$.

Set $\{A_i\} = \mathbf{Generate\ 2}(H, M)$.

Merge. Set $V_j^i = \mathbf{Merge}'(V_{2j-1}^{i-1}, V_{2j}^{i-1}, \{A_i\}, s, k, \xi) \subseteq \mathcal{H}_{[(j-1)2^i+1, j2^i]}$, where k, s are as in Theorem 10 (with $r = 1$) and $\xi = \tilde{\Theta}(n^{-1/2})$.

Final step:

Let K be the unique operator A computed at the last iteration, and $\tau = 10\|H\|\gamma^{-1}\log(1/\delta)$. Choose an orthonormal basis $\{|y_i^{(0)}\rangle\}$ for $V_1^{\log n}$. Repeat for $t = 1, \dots, \tau$:

Set $\{|y_i^{(t)}\rangle\} = \text{Trim}_\xi(\text{Span}\{|Ky_i^{(t-1)}\rangle\})$, for $\xi = \tilde{\Theta}(n^{-1/2})$.

Return the smallest eigenvector $|z\rangle$ of H restricted to $W = \text{Span}\{|y_i^{(\tau)}\rangle\}$.

► **Theorem 14 (Efficient AGSP, (FF)).** *Let H be a local Hamiltonian satisfying Assumption (FF), and $\mathcal{H} = \mathcal{H}_L \otimes \mathcal{H}_M \otimes \mathcal{H}_R$ a decomposition of the n -qudit space into contiguous regions. There exists a procedure $\mathbf{Generate\ 2}(H, M)$ which takes as input*

- A local Hamiltonian H satisfying Assumption (DG),
- A decomposition $\mathcal{H} = \mathcal{H}_L \otimes \mathcal{H}_M \otimes \mathcal{H}_R$ of the n -qudit space into contiguous blocks, and returns MPO representations for a collection of D^2 operators $\{A_i\}_{i=1}^{D^2}$ acting on \mathcal{H}_M such that the following hold:

- $D = 2^{\tilde{O}(\gamma^{-1}\log^3 d)}$
- There is $\Delta > 0$ such that $D^{12}\Delta < \frac{1}{2000}$ and for any $S \subseteq \mathcal{H}_M$ that is δ -viable for $\{|\Gamma\rangle\}$ it holds that $S' = \text{Span}\{\cup_i A_i S\}$ is δ' -viable for T with $\delta' = \frac{\Delta}{(1-\delta)^2}$.
- Each A_i has bond dimension at most $2^{\tilde{O}(\gamma^{-2}\log^5 d)}$.

Moreover, for constant d and $\gamma > 0$ the procedure $\mathbf{Generate\ 2}(H, M, \varepsilon'_M)$ runs in time $n^{(1+o(1))}$.

We note that in the case where M consists of all n qudits the procedure returns a single operator A acting on the whole space. Algorithm 3 is an adaptation of Algorithm 2 to the case of frustration-free Hamiltonians.

► **Theorem 15.** *Let H be a local Hamiltonian satisfying Assumption (FF) and $\delta = n^{-\omega(1)}$. With probability at least $1 - \frac{1}{n}$ the vector $|z\rangle$ returned by Algorithm 3 is such that $|\langle z|\Gamma\rangle| \geq 1 - \delta$. Moreover the algorithm runs in time $O(n^{1+o(1)}M(n))$, where $M(n) = O(n^{2.38})$ denotes matrix multiplication time.*

The proof follows the same outline as that of Theorem 13 analyzing Algorithm 2, and we refer to the full version [2] for details. We note that in [7], Huang gives a very simple, though less efficient, algorithm for this frustration free case, by adding one particle at a time and within each step randomly projecting onto a one dimensional space followed by application of an AGSP.

Acknowledgements. We thank Andras Molnar for comments on an earlier draft of this paper, and Christopher T. Chubb for comments and the permission to include the suggestive pictures representing the tensor network structure of the isometry produced by our algorithms.

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