Efficient approximation of degenerate ground states of gapped spin chains.

The unfrustrated case.

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Abstract

In spite of a plethora of no-go results that prevent classically efficient simulation of quantum systems in general, heuristic methods have seen great success, proving typically efficient in practice. The downside of these heuristic methods is that we lack a rigorous understanding of how, and for which systems, they fail. Provably efficient algorithms – even if practically surpassed by heuristic methods – are of key importance for understanding the true worst-case complexity of simulation. The cutting edge for provably efficient simulation is the ground state approximation of 1D spin systems. Under the assumption of a gap, there exists a provably efficient algorithm for approximation of a unique ground state of such systems; in this thesis we extend this algorithm to work for degenerate systems. This result comes in the wake of a recent degenerate extension of the area law, an important structural bound on the complexity of ground states. In practice this algorithm is no match for heuristic analogues such as the density matrix renormalisation group. However, it does add to the increasing understanding of the systems for which provable efficiency is attainable, and might hopefully lead to a future algorithm that is both provably *and* practically efficient.

Acknowledgements

I would like to thank my supervisor – Steven Flammia – for suggesting this interesting project, as well as the several we attempted before it. I would also like to thank him for significant help in the writing of this thesis, and his guidance more generally throughout the project.

Statement of Student Contributions

The original idea – a degenerate extension of the algorithm by Zeph Landau, Umesh Vazarani and Thomas Vidick (LVV) in Ref. [1] – was suggested by my supervisor Steven Flammia. Much of the early work was based solely on this algorithm, though the improved results of Yichen Huang in Refs. [2, 3] respectively – both of which were published during the project – were also later incorporated into the final algorithm.

The introductions and broad overview of the algorithm given in Sections 3.1, 3.2 and 3.3, as well as extension, bond truncation and final optimisation steps of Sections 3.4.1, 3.4.3 and 3.4.5 respectively, are attributable to LVV. The entire error reduction of Section 3.4.4 and the energetic size-trimming of Section 3.4.2 steps are very similar to those of Huang's improved algorithm, though some of the details surrounding the AGSP that were omitted therein are expanded on in Appendix B. The proofs laid out in Sections 4.1, 4.2, 4.5 and 4.7 are all generalisations of those given by LVV. Similarly the boundary contraction and energetic size-trimming proofs of Sections 4.3 through 4.4 generalise those given by Huang. The details of these proofs – insofar as they are original – is my own work.

These generalisations aside, the main original contribution of this thesis is the orthogonality size-trimming, the procedure of which is laid out in Section 3.4.2 and the associated proofs in Sections 4.4.1 through 4.4.3. This work was also largely my own work, though discussions with Steve were invaluable in ruling out other potential procedures.

The analogy drawn in Section 2.3 to the history of linear programming was made by Steve, and was invaluable in understanding the significance of the project. The idea behind Appendix D and the comparisons to the algorithm of Ref. [4] resulted from discussions with Tobias Osborne.

I certify that this report contains work carried out by myself except where otherwise acknowledged.

Signed:  .....

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Simulations are believed by no one except those who conducted them. Experimental results are believed by everyone except those who conducted them.

– Anonymous

Chapter 1

Introduction

Many physical systems – quantum systems especially – can be exceedingly difficult to construct or manipulate, rendering their direct study impractical. Short of experimental realisation, numerical simulation offers the most direct analytic window into such systems.

In his pioneering paper on the role of computer simulations in physics, Feynman [5] showed that for a general quantum system efficient classical simulation is not possible; such simulations suffer an exponential[1] slow-down. Circumventing this slow-down requires computational power exceeding that of classical hardware: a *universal quantum computer* [6]. In the absence of practical universal quantum computation, classical computers serve as the most powerful available platform for such simulations. As such, the systems which can and cannot be efficiently classically simulated are of significant practical importance. While there may be no hope for the efficiency of arbitrary quantum simulations, we may expect the computationally troublesome states may not be 'natural' in some sense. The idea behind efficient simulation is to tap into this natural computational simplicity to circumvent the inherent complexity of quantum systems. As we will see, this will manifest in two different approaches: heuristic methods and physical constraints.

In this thesis we are going to consider ground state approximation of 1D spin-chains (1D-GSA). For such systems heuristic methods – such as renormalisation techniques – have been used to great success in recent years [7, 8, 9]. In spite of the typical efficiency of these methods however – as we will see later in Section 2.2 – these systems cannot be efficiently[2] simulated in general. This apparent conflict makes 1D-GSA a good test-bed for the construction of provably efficient algorithms which rely on physical constraints instead of heuristics, which will be the main concern of this thesis.

1.1 Heuristic Methods

One way of exploiting the computational simplicity of natural systems is to employ heuristics, often in the form of an ansatz. The advantage of this approach is that heuristics can often be expressed in a way that makes their practical value clear – the disadvantage being that their connection to physical conditions is often more opaque. A non-exhaustive list of commonly used heuristics in the study of various quantum systems is given in Figure 1.1.

A consequence of the unclear connection between a heuristics and the underlying physics is the lack of a rigorous understanding of the systems for which these heuristics work. In spite of this rather significant theoretical down-side, the practical advantages have meant that typically efficient heuristics have been developed which have proven highly effective for many large classes of systems for which no provably efficient algorithms yet exist. Indeed, for the problem of 1D-GSA, heuristic methods had been the only game in town until the recent landmark algorithm of Landau, Vazarani and Vidick [1] which provided the first provably efficient 1D-GSA algorithm.

[1] Unless there exist sub-exponential time solutions to NP-hard problems, which are widely believed not to exist. More explicit results are given in Section 2.2.

[2] Assuming $\mathsf{P} \neq \mathsf{NP}$. We will be more explicit about this in Section 2.2.

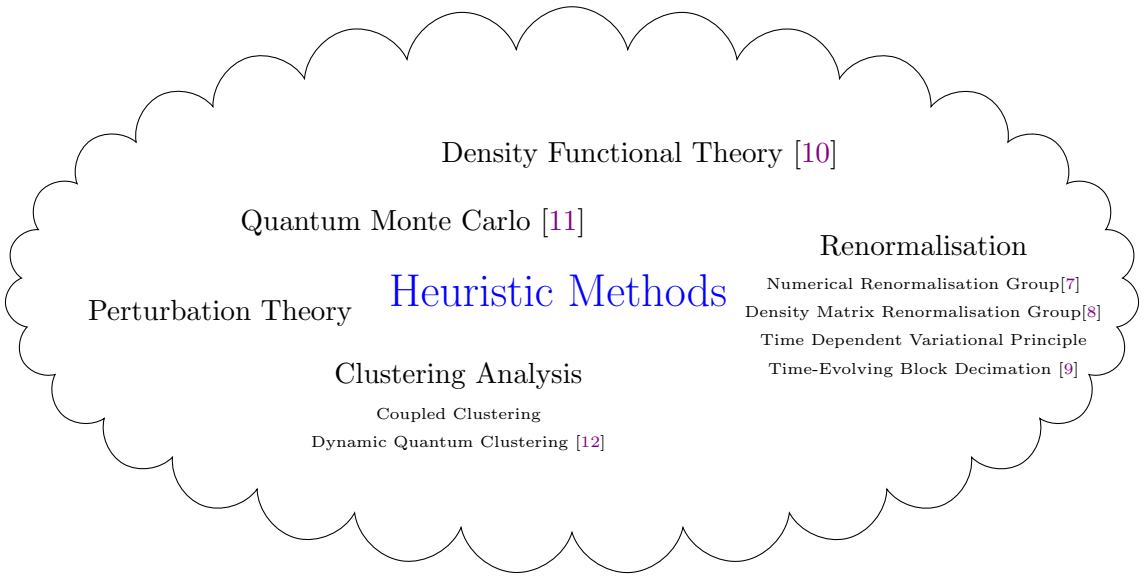


Figure 1.1: Several common heuristic methods for simulating quantum systems.

1.2 Physical Constraints

The more rigorous approach – instead of employing heuristics of unclear interpretation – is to apply constraints to the physical interactions allowed.

The systems we are going to consider are those with local interactions and a spectral gap, the details of which are explored in Sections 2.4 and 2.5 respectively, and their combination in Section 2.6. These two constraints lead to a crucial structural bound – the *area law of entanglement entropy* – which gives an upper bound on the amount of entanglement ground states can exhibit; the details, intuition and history of which is given in Section 2.7. Building on the area law, Ref. [1] provided the first provably efficient stochastic 1D-GSA algorithm for gapped systems. This was recently extended in Ref. [3], giving a *deterministic* algorithm with an improved runtime. Both of these algorithms however only work for systems which possess a unique ground state.

In this thesis we will describe an algorithm which can approximate the ground states of local and gapped 1D systems with constant degeneracy. This result comes in the wake of the recent extension of area law to degenerate systems[3] in Ref. [2]. This algorithm is based on its predecessors Refs. [1, 3], and incorporates ideas from the fields of convex programming, metric spaces and classical constraint satisfaction problems, as well as approximate ground state projectors, an important technical tool for relating the structural and computational features of gapped systems [13, 14].

[3]We will in fact need to use a slightly strengthened form of the area law than has not yet been rigorously proven; more details are given in Section 2.7.

There is a theory which states that if ever anyone discovers exactly what the Universe is for and why it is here, it will instantly disappear and be replaced by something even more bizarre and inexplicable. There is another theory which states that this has already happened.

– Douglas Adams, *Restaurant at the End of the Universe*

Chapter 2

Background

In this chapter we are going to expand on several points from the introduction, and introduce the technical tools that will be needed in our algorithm.

First, to help explore what it means for a heuristic to fail, we are going to consider the Kondo model; a condensed matter system that certain heuristics fail to simulate in an accurate way. With that in mind, we then consider simulation from the perspective of complexity theory, giving more detail as to why neither general systems nor heuristic methods offer any hope for provably efficient simulation. To help explore the significance of heuristic methods and provably efficient algorithms we are going to then look at the history of linear programming, a problem with a very similar history.

Given these background details we will then lay out the two physical constraints – locality and a spectral gap – on which our algorithm will capitalise.

2.1 The Kondo Problem – A case study in heuristic failure

Early measurements of low-temperature metal resistances – most notably gold – were known to exhibit an unexpected minimum, such as those in Figure 2.1. A proposed explanation for this low temperature increase is the presence of magnetic[1] impurities (most likely iron in the case of gold), an interaction known as the *Kondo effect* [15]. Kondo predicted that these sparse impurities cause a logarithmic divergence of the resistance at low temperatures, explaining the minima observed. Whilst this behaviour occurs at low-temperature ($\sim 4K$ in gold/iron), this analysis did not extend to very low temperatures ($\sim 10^{-1}K$), where we would physically expect the impurities to become screened and for the Kondo Effect to be negligible. The total resistance – divided up into the interactions of electrons with other electrons, the lattice, and the spin impurities respectively – was predicted to be of the form

$$R = R_0 + \underbrace{aT^2}_{\text{Electron}} + \underbrace{bT^5}_{\text{Lattice}} + \underbrace{c_m \log \frac{\mu}{T}}_{\text{Spin}} .$$

The heuristic used to predict this was *perturbation theory*[2]. Central to this is the idea of a perturbative expansion: given an impurity system with some property P and some parameter impurity density ρ, then this property can be expanded into a formal power series.

$$P(\rho) = P_0 + \rho P_1 + \rho^2 P_2 + \cdots .$$

If the impurities are sparse, then truncation of this expansion should well-approximate the true value. For small ρ we would expect that the nth order truncation $P^{(n)}$ would have an error on the order of $\delta P^{(n)}$ where

$$P^{(n)} := P_0 + \rho P_1 + \cdots + \rho^n P_n \qquad \delta P^{(n)} := \left| P(\rho) - P^{(n)}(\rho) \right| \sim \rho^{n+1} P_{n+1} .$$

[1] Spin-1/2 particles specifically, though the behaviour is general.

[2] The second Born approximation specifically.

The magnetic impurities in the Kondo model however exhibit asymptotic freedom; as the system is cooled they bond strongly with one of the conducting electrons to form a non-magnetic bound state. This manifests as the coupling terms P_1, P_2, ... diverging at low-temperatures, causing all of the perturbation errors to diverge as well, even for sparse impurities – this is why Kondo's analysis failed below a certain temperature. As a result the error of any finite-order perturbative approximation can always be made to surpass any error threshold for sufficiently low temperatures.

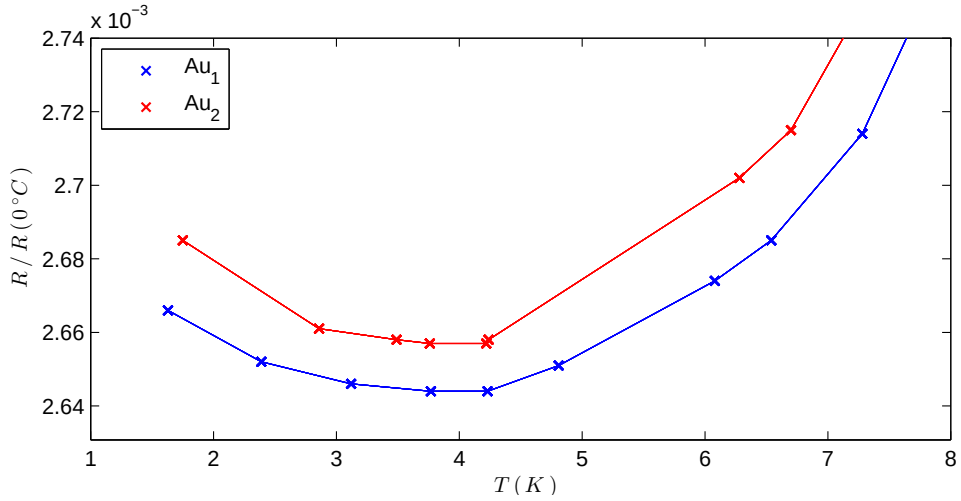


Figure 2.1: The low-temperature resistance of two gold samples [16], exhibiting a minima likely caused by the Kondo effect of iron impurities.

This inherently non-perturbative behaviour made the low-temperature Kondo model inaccessible to perturbative simulation. The problem of extending simulations all the way to absolute zero, and overcoming the non-physical divergence given by perturbation theory, is termed the *Kondo problem*. Due to the ubiquity of perturbative techniques in condensed matter simulations at the time, this problem served as a notoriously difficult test-case for the development of non-perturbative simulations.

2.2 Computational complexity

Whilst restricting to ground state approximation of 1D spin-chains may seem far more trivial than more general simulation, as we shall see it retains much of the computational complexity. This can be formalised in terms of complexity classes which are not believed to possess efficient solutions [17]. Even imposing the restriction of locality for example still leaves this problem far too general to allow efficient approximation. There are known examples of spin-1/2 systems which are combinatorially[3] 5-local [18] and 3-local [19] for which calculating their ground state energy is QMA[4]-complete, a class of problems not believed to be efficiently solvable, even on a quantum computer. Restricting further to geometric locality interactions has the same result, the 2-local qubit Hamiltonian problem on a square lattice still being QMA-complete [20]. As such we will need to restrict our system further, motivated by the nature of physically realistic systems. Whether or not such non-trivial assumptions exist is not immediately clear. The two fields of quantum Hamiltonian complexity theory and the state of previously mentioned heuristic methods shine some light on this, but seem to tell two very different stories.

2.2.1 Quantum Hamiltonian Complexity Theory

Studying this conjecture from the perspective of quantum complexity theory is quite dissuasive, with heavy restrictions on the geometry, topology, and interactions still not mitigating the problematic computational complexity.

[3] Meaning that interactions only act on a constant number of spins.
[4] Quantum Merlin-Aurthur, the quantum analogue of NP.

There exist two-body Hamiltonians whose ground states are capable of universal quantum computation [21, 22], rendering their approximation QMA-complete. Further topological restrictions to 1D local[5] systems still leaves approximation QMA-complete [23, 24], even if translation invariance is enforced [25]. Things are looking bad for our desired classical simulability.

2.2.2 Heuristic Methods

Whilst complexity theory seems to yields only bad news, we now return to the heuristic methods that raised the possibility of such efficient algorithms in the first place.

For the problem we are considering – ground state approximation of a spin-chain – techniques based on renormalisation groups offer the state-of-the-art performance both in terms of efficiency and the class of systems capable of being simulated. Renormalisation techniques were introduced into the field of condensed matter simulation in an attempt to address inherently non-perturbative systems such as the Kondo problem of Section 2.1. The *Numerical Renormalisation Group* (NRG) [7] was the first such renormalisation algorithm, designed to approximate the ground states of the Kondo model. The NRG was in turn generalised to a larger class of quantum impurity problems; a detailed review of NRG can be found in Ref. [26]. NRG itself was rather specialised, but the general renormalisation approach it introduced is its main legacy.

The next big advancement was the *density matrix renormalisation group* (DMRG) [8], a more general heuristic for 1D-GSA. DMRG and its derivatives stand as the state-of-the-art in 1D simulation methods. Broad reviews of the topic can be found in Refs. [27, 28] and a review within the modern matrix product state formalism (see Section 2.7.2) in Ref. [29]. Whilst the original form of DMRG was a ground state approximation algorithm (the main concern of the thesis), the formalism has since been extended to allow for general time evolution of low-temperature systems via the *time evolving block decimation* (TEBD) formalism [9, 30], the *infinite time evolving block decimation* (iTEBD) formalism [31] and directly [32]. There has been work towards 2D and 3D extensions of DMRG [33], but the algorithm is most naturally expressed within the matrix product state (Section 2.7.2) formalism that is most effective in one dimension.

The practical efficiency of DMRG for a wide-range of non-trivial one dimensional systems serves as a rebuttal to the apparent forecast of quantum Hamiltonian complexity theory, reviving the possibility of provably efficient simulation of these systems. One is tempted to ask the question as to whether DMRG, or some modification thereof, may be a viable candidate for just such a procedure. The down-side of DMRG and its offspring – at least from a theoretical perspective – is that they are inherently heuristic in nature and are *provably not efficient*, at least in the worst case. There exist ground states of 1D systems for which DMRG is required to solve NP-hard problems [34], and cannot even be approximated efficiently[6]. This doesn't however – as we shall see – rule out the possibility of a provably efficient algorithm.

The two main features of DMRG that provably efficient algorithms borrow are both the general variational approach, and the matrix product state representation; we will explore the latter of these in Section 2.7.2.

2.3 Linear Programming

Given that heuristic methods are far more practically efficient than any provably efficient analogue, one may wonder why we care about such algorithms. This question is best answered by example, through the history of linear programming.

Given real vectors $\mathbf{c}$ and $\mathbf{b}$ and a real matrix A, linear programs (LP) [35] are optimisations over

[5] Geometric locality, meaning interactions have a finite range.

[6] Assuming P≠NP.

a real vector $\mathbf{x}$ that take the standard form

$$\begin{aligned} \text{maximise} \quad & \mathbf{c}^T\mathbf{x} \\ \text{subject to} \quad & A\mathbf{x} \leq \mathbf{b} \\ & \mathbf{x} \geq 0\,. \end{aligned}$$

Much like the problem of 1D-GSA, the first step towards an efficient LP algorithm came in the form of a heuristic method, known as the *simplex method* [36]. Much like perturbation theory and DMRG for 1D-GSP, the simplex method is known to fail for certain linear programs, suffering from a behaviour known as *stalling* [37]. Indeed there are programs for which the simplex method is known to take exponentially long in the input size [38, 39].

The first provably efficient algorithm developed was the *ellipsoid method* [40]. In spite of this efficiency, it is by no means a practical algorithm, having a best-case and average-case efficiency far worse than the simplex method. It is this algorithm that the current provably efficient 1D-GSA algorithms – including this thesis – are analogous to.

The significant next step, for which 1D-GSA has no analogue as yet, is Karmarkar's algorithm [41, 42]. This algorithm built on the provable efficiency of the ellipsoid method, but also achieved a practical efficiency comparable to simplex; indeed current state-of-the-art interior-point methods – descendents of Karmarkar's algorithm – are known to now be at least as efficient as the simplex method [43].

Whilst the provably efficient algorithm laid out in this thesis may not be as efficient as DMRG and other heuristics in practice, it might lead to an algorithm – like Karmarkar's Algorithm – that shares the best of both worlds: practical *and* provable efficiency even in the worst case.

2.4 1D Locality

The first big restriction we will be making is considering only one-dimensional spin chains. Geometrically this will mean that we can consider the spins within a system placed on a line, labelling these spins by $1, \ldots, n$. On top of this we shall also restrict the topology of the system, only allowing for geometrically local interactions with a constant and finite interaction length. By blocking together spins and rescaling the local interactions, each term of the Hamiltonian can be taken to only act on nearest-neighbours, be non-negative, and have a unit bound norm – all without loss of generality. Specifically this will mean the Hamiltonian is of the form

$$H = \sum_{i=1}^{n-1} H_i \qquad\qquad 0 \leq H_i \leq 1$$

where H_i acts only on the i and $i+1$ spins of some fixed finite dimension d (qudits).

Finding the ground state of a local Hamiltonian is the quantum analogue of the classical constraint satisfaction problem (CSP)[7] – indeed a CSP could be expressed as finding the ground state of a classical Hamiltonian. Much of the analysis of 1D CSP can thus be carried over to the local Hamiltonian problem [18, 44]. Whilst care has to be taken to get around uniquely quantum features such as entanglement, noncommutativity, and the marginal problem [45, 46], techniques originally developed in the context of 1D CSP can be utilised in the construction of efficient ground state algorithms.

The CSP is given by a set of Boolean functions B_i, analogous to the local Hamiltonian terms. A solution to this problem is given by a state which satisfies all of these Boolean conditions. This is a specialised case of the (classical) local Hamiltonian problem where $H_i = 0$ for $B_i = \text{true}$ and $H_i > 0$ for $B_i = \text{false}$. A Hamiltonian for which a global minimum is everywhere a local minimum, such as this, is termed *unfrustrated* or *frustration-free*. This problem can be relaxed into a more general CSP in which only a fixed number of constraints need be met (analogous to a frustrated local Hamiltonian problem) and a decision problem asking whether a given number of constraints can be met (analogous to a ground energy problem).

[7] Strictly speaking it is a *weighted* CSP if the Hamiltonian is frustrated.

A general CSP, defined on an arbitrary finite domain, is NP-complete [47]. As this is a specialised case of the local Hamiltonian problem, this removes any hope for solving such problems without further restrictions. The 1D local restriction of the CSP is however in P, with efficient algorithms known to exist [48, 47].

In 1D, the technique that allows for this efficient solution is known as *decoupling*. The idea behind decoupling is to split the problem along a cut, say across $(j, j+1)$. The problem of solving the CSP for the entire systems can now be reduced to solving the CSP for both the $0 \leq i \leq j$ and $j+1 \leq i \leq n$ half-chains, and then combining these in a way that satisfies the B_j constraint across the cut. Using such decoupling the problem can be iteratively solved by combining solutions on small domains to yield solutions on larger domains.

Strict decoupling in this way however does not hold for the local Hamiltonian problem due to entanglement across the cut. Classically, states always factor into unique states on each subsystem, allowing states to be constructed in a piecewise fashion. Entanglement however means that quantum systems needn't factor in this way, and as such there does not always exist a global state consistent with a given set of locally specified states. The problem of constructing such a consistent global state is known as the quantum marginal problem (QMP) [45, 46].

This is where the previously mentioned structural bound comes into play. If ground states were to exhibit an arbitrarily large amount of entanglement, then the QMP would be insurmountable. As we shall see however this is not the case; ground states can only exhibit a small amount of entanglement, allowing for many classical intuitions to approximately hold for them. These ground states exhibit an approximate form of decoupling, which will allow us to use a technique known as *boundary contraction* (see Section 4.3) to construct full-chain solutions out of half-chain solutions.

Whether or not efficient ground state algorithms exist in more than one dimension is an open problem. Due to the existence of efficient 1D CSP algorithms – as well as the practical efficiency of 1D heuristic methods (DMRG/TEBD/iTEBD) – we will restrict ourselves to the 1D case for the purposes of this thesis.

2.5 Spectral Gap

Entanglement – and in turn the exponential growth in the variables required to represent an arbitrary amount of it – is one of the main sources of computational difficulty of quantum systems. Any class of systems on which efficient simulations are possible must therefore posses a structural bound on the amount of entanglement that they are able to exhibit. Indeed, the existence of such a structural bound for gapped and local 1D Hamiltonians is key to the efficiency of our algorithm.

Intuitively the concept of an approximate ground state and low-energy state may seem interchangeable. Whilst a lower bound on the ground space overlap does imply a non-trivial upper bound on the energy, the opposite is only true below the first-excited energy. To utilise this intuition our algorithm will need to stay within this energy range: between the ground and first-excited energies. As such the size of this energy range is rather significant.

Specifically, define the *spectral gap* of a system to be

$$\Delta E := E_1 - E_0$$

where E_i is the ith excited energy level[8]. If we then have a state $|\psi\rangle$ with energy bounded by E, then decomposing this state into ground and excited components gives a lower bound on the ground space overlap

$$\left|\langle \Gamma | \psi \rangle\right|^2 \geq 1 - \frac{E - E_0}{\Delta E}$$

for some ground state $|\Gamma\rangle$. For this result to be non-trivial we require that the energy of the state is within the gap, $E < E_0 + \Delta E$. If this gap is allowed to shrink as the system grows, then this narrow spectral window in which we can operate narrows as well. As such we will define families of systems

[8] Taking into account degeneracy, such that $\Delta E > 0$.

which retain a gap in the thermodynamic limit – for which the gap is lower bounded by a constant $\Delta E = \Omega(1)$ – as *gapped systems*[9].

The fact that low-energy states are also approximate ground states for such systems opens the door to a recently developed technical tool which has proven to be a fruitful connection between structural and computational results [49, 50] known as an *approximate ground state projector*.

2.5.1 Approximate Ground State Projectors

So far we have talked about the physical constraints we need to make 1D-GSA tractable, but not how we will go about performing ground state approximation. To this end we require an operator capable of taking a state that might already be close to the ground space and pushing it closer.

The most powerful such operator we could imagine is an exact ground state projector (EGSP); an operator P such that $P|\psi\rangle$ is a ground state for all state $|\psi\rangle$. Such a projector would take the form

$$P = \sum_i |\psi_i\rangle\langle\psi_i|$$

where $\{|\psi_i\rangle\}$ is an orthonormal set of ground states. As such an EGSP is just as complicated as an exact ground state, meaning we can neither construct nor represent it in an efficient manner in general.

Whilst a EGSP would give us access to *exact* ground states, we only need to achieve ground state *approximation*, and so the operator we need is an *approximate* ground state projector (AGSP). Instead of acting as the zero operator on the domain orthogonal to the ground space – which is the case for a EGSP – an AGSP simply has a small bounded norm. In essence this means that instead of entirely destroying any excitation components, it shrinks them significantly. Applying such an AGSP might not yield an exact ground state, but it will amplify the ground space overlap.

Whilst the transition from EGSPs to AGSPs gives us the wiggle-room we need for these operators to be efficiently represented and constructed, we haven't yet discussed how one would construct them; this is where the gap comes in. The Hamiltonian is the object that defines what is and is not a ground state, so we may expect that AGSPs can be constructed out of the Hamiltonian. If a system is gapless then there exist very low energy states with no ground-state overlap, making them difficult to differentiate. If however the Hamiltonian is indeed gapless then it alone is sufficient to construct an AGSP. The construction of an AGSP is exemplified by the concept of *imaginary time evolution*. Consider an AGSP A which is defined as the evolution of a system for a time $i\tau$. Taking $U(t)$ to be the time evolution operator we have

$$A = U(i\tau) = \exp(-H\tau)$$

Taking the ground energy of H to be 0 for simplicity, we can see that A fits the definition of an AGSP, A having a norm bounded by $\exp(-\Delta E\,\tau)$ orthogonal to the ground space. The AGSP we will in fact use is slightly more complicated; a linear combination of real time evolution operators in fact, but this gives the idea of what an AGSP is. A more detailed history of AGSP constructions is given in Appendix B.

2.6 Gapped and local systems

Ground states of gapped and local systems exhibit two important properties that allows the entanglement of their ground state to be bounded.

The first result is known as the *Lieb-Robinson bound* [51]. It states the locality of a Hamiltonian translates into an approximate light-cone type behaviour, with observables outside of each other's light-cones approximately commuting[10], up to exponentially small corrections. This light-cone is given by the so-called Lieb-Robinson velocity v_{LR}. The specific bound is

$$\|[A, B]\| \leq 2e^{-c(d - v_{LR}t)} \|A\| \|B\| \tag{2.1}$$

[9] Here $\Omega(f(x))$ denotes an asymptotic *lower* bound, compared to $\mathcal{O}(f(x))$ which denotes an upper bound.

[10] The relativistic light-cone can be expressed as the commutation of space-like separated observables.

where d and t are the distance and time separating the two measurements, and c is a constant independent of the measurements. In quantum-field-theoretic terms this is analogous to a speed of sound that some local interactions exhibit. A short review of the Lieb-Robinson bound can be found in Ref. [52], lecture notes on its relationship to locality in Ref. [53], and its relevance in the context of simulation in Ref. [54].

The second result is the *exponential decay of correlations* [55]. It states that the correlation between two local observables A and B, acting on the ground state of a local Hamiltonian system, exhibits an exponential decay with characteristic length ξ, both given by

$$|\langle AB\rangle - \langle A\rangle\langle B\rangle| \leq e^{-d/\xi}\,\|A\|\,\|B\| \quad , \quad \xi := \frac{2v_{LR}}{\Delta E}\,. \tag{2.2}$$

For gapped systems $\Delta E = \Omega(1)$ and so $\xi = \mathcal{O}(1)$, i.e. the correlation length is bound from above by a constant. In quantum-field-theoretic terms this is analogous to the bounded interaction range that fields exhibit in the presence of a mass gap; indeed, due to this relationship gapped quantum phases were historically dubbed *massive* [56] by way of analogy.

Both of these results can be interpreted as an 'informational locality' of these ground states. As a result we may intuitively expect regions separated by large distances – relative to the correlation length ξ – to be only weakly entangled.

2.7 Area Law

Now we return to our biggest roadblock: representing states of bounded entanglement. A bound on the entanglement of ground states to local gapped Hamiltonians, or at least a bound on the entanglement required to well-approximate such states, is therefore a necessary first step towards an efficient algorithm to find them.

The entanglement of a quantum system is a measure of the amount of information of a state not contained in the individual parts of that state. Starting with the state (density operator) of a system, the state restricted to a subsystem – the so-called *reduced* density operator – can be found by partial tracing out all parts of the state outside of that subsystem. Taking a pure state, the entropy of a reduced density operator on some region – a measure of how mixed that state is – gives a measure of the entanglement between that region and its complement. Entropies in this context are specifically referred to as *entanglement entropies*. The *Rényi entropy* – an important family of entropies – is defined for a given reduced density operator ρ_A as

$$R_\alpha(\rho_A) := \frac{1}{1-\alpha}\log\,\mathrm{Tr}\,(\rho_A^\alpha)\,,$$

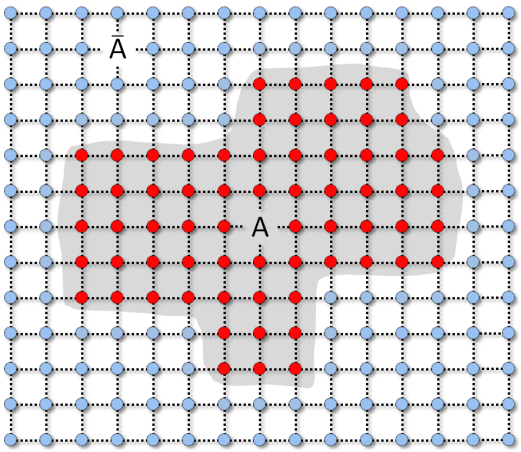
where $\alpha \geq 0$ controls the relative weighting of various eigenvalues. Included in this family are both the regular *Von Neumann entropy* S and the *Hartley entropy* R_0, known as the entanglement entropy and the log of the entanglement rank respectively in this context.

$$R_1 = S = -\,\mathrm{Tr}\,(\rho_A\,\log\rho_A) \quad , \quad R_0 = \log B = \log\big(\mathrm{rank}(\rho_A)\big)\,.$$

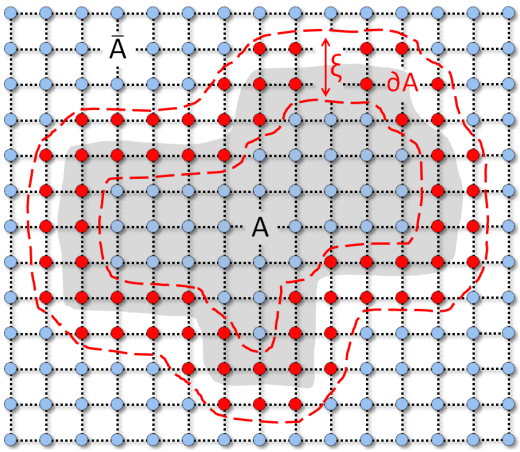
In general the entanglement entropy between a region A and its complement $\bar{A}$ can scale according to a *volume*[11] *law* $S \leq \mathcal{O}(|A|)$ as shown in Figure 2.2(a). Given the informational locality described in above in Section 2.6 however, we might expect a picture more along the lines of Figure 2.2(b), and an associated *area law* $S \leq \mathcal{O}(|\partial A|)$.

An area law of entanglement is conjectured for several large classes of quantum systems: those with statistical properties like an exponential decay of correlations [57, 58], thermal properties such as a polynomial-decaying specific heat [59], and – most importantly for our purposes – ground states of gapped and local systems [60]. A further highly generalised form of the area law – for gapped and local systems defined on arbitrary graphs – was also long conjectured, though a counterexample

[11] 'Volume' and 'Area' here are used in their abstract sense, volume referring to the quantity of spins in a region and area to the quantity around the boundary. In 1D, for a simply connected region, the 'volume' is the length and the 'area' is a constant.



(a) A volume law, the scaling of a general state.



(b) An area law, scaling believed to be typical of local and gapped ground states.

Figure 2.2: The scaling of entanglement entropy between regions A and $\bar{A}$, proportion to the number of red spins.

to this has recently been found [61]. Analogous results have also arisen in other contexts, such as the *Hawking-Bekenstein entropy* of a black hole [62] – a connection first made in Ref. [63] – and the *holographic principle* [64, 65] in string theories and the study of quantum gravity. See Ref. [60] for a detailed review of the area law.

2.7.1 State of the art

A longer history of the proofs of the area law for 1D gapped systems, as well as a sketch of the methods used, is given in Appendix A. The best current area law result is given in Ref. [2]. Consider a constant-degeneracy, 1D local, gapped system – with a gap lower bounded by $\epsilon = \Omega(1)$. Then across every cut there exists a ground state which not only obeys an area law, but a *Rényi* area law, with an entropy bounded by

$$R_\alpha \leq \tilde{\mathcal{O}}(\alpha^{-3}\epsilon^{-1}) \qquad \forall \alpha \in (0,1]\,,$$

which has precisely the $\mathcal{O}(\xi)$ upper bound on S we intuitively expected from Figure 2.2(b), up to logarithmic corrections.

A von Neumann area law alone is not suitable for our purposes – there exist states with such a bound that cannot be efficiently represented [66]. The extension to a Rényi area law has an important corollary[12] which does allow efficient representation of approximate ground states: for any given cut there exists an approximate ground state with inverse-polynomial error and an entanglement rank

$$B \leq \exp\left(\tilde{\mathcal{O}}\left(\epsilon^{-1/4}\log^{3/4} n\right)\right)\,.$$

2.7.2 Matrix Product States

An important requirement for the time efficiency of an algorithm is spatial efficiency, so if we want to show an algorithm lies in P we must first have that it lies in PSPACE (since P $\subseteq$ PSPACE). To this end we require a state ansatz which allows for states to be represented in a manner that is both spatially efficient, and allows for computations to be performed efficiently.

The first step towards such an ansatz came from Affleck, Kennedy, Lieb and Tasaki in their analysis of the eponymous anti-ferromagnetic AKLT model [68]. Their specialised *valance bond state* construction was in turn generalised to so-called *finitely correlated states* (FCS) [69]. This construction

[12] Whilst Ref. [66] shows that this corollary holds for any state with a Rényi area law, the knowledge that this corollary holds for 1D gapped ground states – as is mentioned in Ref. [67] – pre-dates the proof of such an Rényi area law, and was proven independently.

however is rather ad hoc, leaving the physical relevance of their validity in any approximation rather opaque. One feature that all finitely correlated states do possess – and that a typical state does not – is various bounds on the level of entanglement able to be represented by the state [70], a feature we desire in our state ansatz. Ideally however we would like to tip this procedure on its head: start from desired entanglement bounds and form an ansatz capable of representing states subject to such bounds.

A similar problem – the efficient approximation of members of exponentially large vectors spaces – arises commonly in tensor analysis. Around the same time as the FCS construction, an ansatz known as the *tensor train decomposition* (TTD) arose in this field [71].

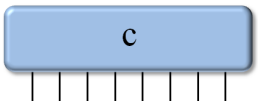
Similar to FCS arising from a generalisation of the techniques used in the AKLT analysis, deeper analysis of the DMRG and similar renormalisation techniques also yielded a general class of ansatz: *matrix product states* (MPS). Indeed when considered in the correct way, MPS can be considered as special cases both of FCS [72] and TTD [73].

The idea behind the MPS construction is to take a general state and split it into its local contributions. The relationships between these local terms then will be indicative of the entanglement between the two regions. By then truncating the complexity of these inter-relationships the number of variables required can be made efficient, at the cost of only representing bounded levels of entanglement. In this manner we can translate entanglement bounds into an efficient representation.

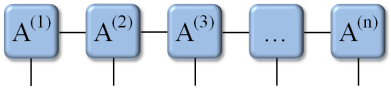
A general spin-chain state is of the form

$$|\psi\rangle = \sum_{i_1,\cdots,i_n=1}^{d} c_{i_1,\cdots,i_n} |i_1, \cdots, i_n\rangle$$

In tensor network notation[13] this general state – or at the very least the coefficients thereof – can be represented



where each vertical free leg represents a free index of $c_{i_1,\cdots,i_n}$. We wish to now break this tensor into parts localised to each spin; this is done by performing *Schmidt decompositions* – a form of low-rank approximation [74] equivalent to singular value decomposition – across every cut. This yields a state of the form



where the horizontal connections now represent contracted tensorial indices; the titular matrix products. The number of values these horizontal indices take is known as the *bond dimension* B. For an arbitrary state an exponential bond dimension is required. The total number of variables required to represent such a state is dnB^2, so this representation is generally inefficient. The bond dimension however – as the choice of pronumeral may suggest – coincides with the entanglement rank of these states. Truncating the bond dimension to be at most polynomial in n, such a decomposed state forms our desired ansatz: a *matrix product state*.

As ground states – and more to the point their approximations – do exhibit similarly bounded levels of entanglement, this allows for states to be both efficiently represented [75, 66] and for efficient calculations to be performed with them [66]. As such the ground state approximation problem is narrowed to PSPACE, and further to NP in the unfrustrated case.

[13] Known as Penrose graphical notation in different contexts.

If in physics there's something you don't understand, you can always hide behind the uncharted depths of nature. You can always blame God. You didn't make it so complex yourself. But if your program doesn't work, there is no one to hide behind. You cannot hide behind an obstinate nature. If it doesn't work, you've messed up.

– Edsger Dijkstra

Chapter 3

Algorithm

In this chapter we will lay out the algorithm itself, as well as motivate each of the steps taken. We will state various bounds on the result of each step, but will leave the proofs of these bounds for Chapter 4. First the main result:

Theorem 1 (Main Result)**.** *Let H be constant-fold degenerate, unfrustrated, n-qudit, 1D local, gapped Hamiltonian, with a gap lower bounded by a constant ϵ. There exists an algorithm which returns an orthonormal set of states – represented as MPS – each of which has a $1-\eta$ overlap with the ground space. The run-time is $T = n^{\mathcal{O}(1/\epsilon)}$ for $\eta^{-1} = n^{\mathcal{O}(1)}$, and $T = n^{\mathcal{O}(1)}$ for $\eta^{-1} = n^{o(1)}$.*

3.1 Viable sets

The linchpin of our algorithm, as well as those of Refs. [1, 3] which pre-date it, is the concept of a *viable set*, and the construction thereof. For a set of states defined on a given half-chain[1] to be viable, there must exist desired *witnesses* – these are approximate ground states – and the reduced witness states on that half-chain must lie in the span of that set. In essence this means a viable set is one which captures the 'local part' of an approximate ground state.

Definition 3.1.1. (Viable Set) For a g-degenerate, n qudit Hamiltonian, with a gap lower bounded by ϵ, a set of states S is $(i, s, b, \delta$ or $\Delta)$-viable if:

- The states in S are supported on the first i spins of the system; $S \subset (\mathcal{C}^d)^{\otimes i}$.
- The cardinality is bounded $|S| \leq s$.
- Each state in S is represented by an MPS with bond dimension at most b.
- There exists an orthonormal set of g witnesses that either have ground space overlap at least $1-\delta$ *or* energy at most $\Delta\epsilon$ (depending on the context). The reduced density operators of these witnesses must be supported on Span S.

The parameter i simply controls the physical scope of the set – growing i whilst keeping all other parameters under control will be the main goal of our algorithm. The parameters s and b control the number of variables required to represent S; $ids b^2$ complex numbers in total. To ensure various forms of computations can be efficiently performed with S, we will require $s, b = \mathsf{poly}(n)$[2] at all times. The parameters δ and Δ are measures of the quality of the witnesses. As discussed in Section 2.5, these two measures are – to a limited extent – interchangeable for gapped systems, though converting between these has an associated overhead. By allowing for either measure to be used in a contextual manner, we avoid unnecessary incursions of this overhead, streamlining some parts of the algorithm.

[1] Half-chain here referring to the first i spins, up to the current point in the algorithm.

[2] Upper bounded by a polynomial in n, without specifying the ϵ-dependence.

Lemma 3.1.2 (Interchangeability of δ and Δ[1, 3])**.** *For some* $|\Gamma\rangle \in G$

$$\begin{aligned} \langle v|H|v\rangle \leq \Delta\epsilon \quad &\implies \quad |\langle v|\Gamma\rangle| \geq 1-\Delta \\ |\langle v|\Gamma\rangle| \geq 1-\delta \quad &\implies \quad \langle v|H|v\rangle \leq \delta(2-\delta)n \leq 2\delta n \end{aligned}$$

which allows us to convert between the two measures of viability

$$\begin{aligned} (\cdot,\cdot,\cdot,\Delta)\text{-viable} \quad &\implies \quad (\cdot,\cdot,\cdot,\delta=\Delta)\text{-viable} \\ (\cdot,\cdot,\cdot,\delta)\text{-viable} \quad &\implies \quad (\cdot,\cdot,\cdot,\Delta=2n\delta/\epsilon)\text{-viable}\,. \end{aligned}$$

3.2 Structure

The big-picture structure of the algorithm is a construction of a $(n, \mathsf{poly}(n), \mathsf{poly}(n), \mathcal{O}(\eta))$-viable set. If such a set can be constructed, then its polynomial size will allow for the Hamiltonian to be efficiently optimised on it in the form of a convex optimisation. This will allow for the witnesses to be extracted from the set, yielding the desired approximate ground states.

To construct this set, a $(i, pp_1, pp_2, \Delta = c\epsilon^3)$-viable set will be constructed for each i, with a more powerful final iteration giving a $(n,p_0p_1,p_0p_2,\Delta = \eta/3)$-viable set. The specific viability bounds for each iteration, as well as the stages within the ith iteration, are shown in Table 3.1, below which the scaling is also given for the various polynomials contained within.

It only remains now to explicitly specify how to iterate over each spin. This requires four stages, each of which adjusts a viability parameter in turn as shown by the red terms in Table 3.1. By explicitly laying out the ith and nth iterations, we will prove the validity of our algorithm inductively, from the starting set $S_0 = \{1\}$.

Stage	i	s	B	δ	Δ
Iteration 0	0	1	0	0	0
Iteration 1	1	pp_1	pp_2	$c\epsilon^3$	$c\epsilon^3$
	⋮	⋮	⋮	⋮	⋮
Iteration $i-1$	$i-1$	pp_1	pp_2	$c\epsilon^3$	$c\epsilon^3$
Iteration i:					
Extension	i	dpp_1	pp_2	$c\epsilon^3$	$c\epsilon^3$
Size Trimming	i	p_1	$dp^2p_1p_2$	$1/100$	$1/100$
Bond Truncation	i	p_1	p_2	$1/4$	$n/2\epsilon$
Error Reduction	i	pp_1	pp_2	$c\epsilon^3$	$c\epsilon^3$
Iteration $i+1$	$i+1$	pp_1	pp_2	$c\epsilon^3$	$c\epsilon^3$
	⋮	⋮	⋮	⋮	⋮
Iteration $n-1$	$n-1$	pp_1	pp_2	$c\epsilon^3$	$c\epsilon^3$
Final Iteration	n	p_0p_1	p_0p_2	$\eta/3$	$\eta/3$

$$p(n) = n^{\mathcal{O}(1)} \qquad p_1(n) = 2^{2^{\mathcal{O}(1/\epsilon)}}$$
$$p_0(n) = (1/\eta)^{\mathcal{O}(1/\epsilon)} \cdot (n/\eta)^{\mathcal{O}(1)} \qquad p_2(n) = n2^{\mathcal{O}(\epsilon^{-1/4}\log^{3/4} n)}$$

Table 3.1: Viability parameters throughout the algorithm. Green indicates the desired parameter in each step, grey the weaker of the two quality parameters, as given by Lemma 3.1.2. The four polynomials below the table are those involved in the scaling of the viability parameters.

3.3 Notation

As described in Section 2.4 we consider Hamiltonians of the form

$$H = \sum_{i=1}^{n-1} H_i$$

where H_i acts non-trivially only on the i and $i+1$ spins. As well as assuming nearest-neighbour interactions, without loss of generality we can scale and offset these terms such that $0 \leq H_i \leq \mathrm{Id}$, with the first inequality being tight. We are specifically going to be considering unfrustrated systems, for which the ground energy is 0, i.e. $\cap_i \ker H_i \neq \emptyset$. For simplicity we are going to be considering a two-fold degenerate Hamiltonian, though the algorithm easily generalises to a constant-fold degeneracy. We are going to take the positive constant ϵ to lower bound the spectral gap, i.e. $H^2 \geq \epsilon H$.

Throughout the algorithm we will use the constant $c := 10^{-14}$, and will require that $\epsilon \leq 3000$. As ϵ is only required to be a *lower bound* on the gap, this assumption can be made without loss of generality.

3.4 Procedure

Suppose we start with a set S_{i-1} which is $(i-1, s, b, \Delta = c\epsilon^3)$-viable.

3.4.1 Extension

The first step is to extend this set onto the next spin. The simplest method of extension is to simply take a tensor product with the computational basis on the next spin.

Algorithm Step 1: Extension

Take $\{|j\rangle\}$ to be the computational basis of the local Hilbert space of the ith qudit $\mathcal{H}_i \cong \mathbb{C}^d$.
Return $S_i^{(1)} := \{|s\rangle \otimes |j\rangle \;|\; \forall\, |s\rangle \in S_{i-1},\; 1 \leq j \leq d\}$.

Claim 1 (Proof in Section 4.2)**.** *The set $S_i^{(1)}$ is $(i, ds, b, \Delta = c\epsilon^3)$-viable.*

As a result this extension comes at a multiplicative cost in the cardinality, and no cost in error. To prevent a subsequent exponentially growing cardinality, a size-trimming step is required. This also happens to be the step that requires the most modification to accommodate degeneracy.

3.4.2 Size Trimming

The size-trimming optimisation is where we employ the *approximate decoupling* described in Section 2.4.

Firstly split the Hamiltonian into three pieces across the cut: the left and right Hamiltonians $H_L := H_1 + \cdots + H_{i-1}$ and $H_R := H_{i+1} + \cdots + H_n$, as well as the overlapping term H_i. The idea is that for a ground state – a minima of the Hamiltonian – the expectation values of the left and right Hamiltonians should also be low[3]. As a result we could expect that by minimising the left-Hamiltonian – in some way guaranteed to be consistent with a witness – we can generate a viable set. Moreover the cardinality of viable set $S_i^{(2)}$ generated in this way will be independent of the input set $S_i^{(1)}$, so this process will perform the desired size-trimming.

For our purposes we are going to be considering unfrustrated systems in which ground states not only possess left/right-Hamiltonian expectation values which are *low*, but in fact zero. Such unfrustrated systems exhibit *exact decoupling*, which is more in line with the classical CSP analogue.

[3] More explicitly this manifests as the *truncation lemma* of Refs. [3, 67]. The unfrustrated version of the truncation lemma however is far simpler, and given in Lemma 4.3.3

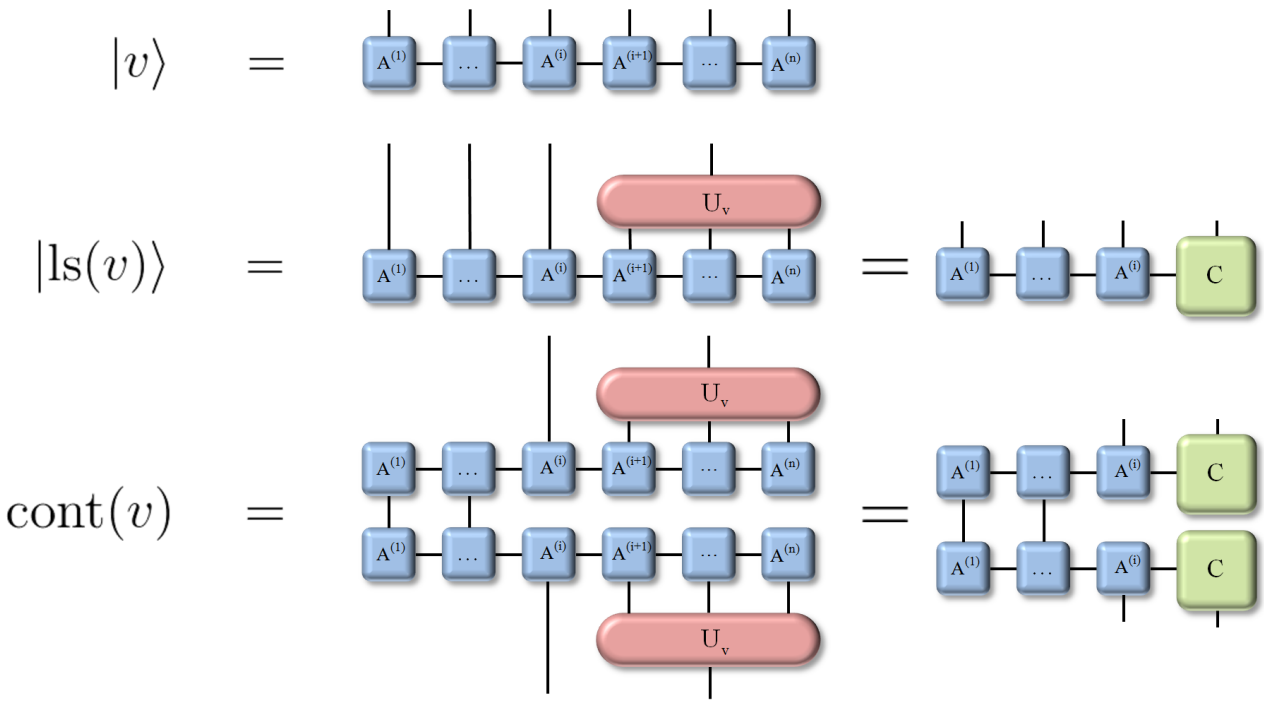


Figure 3.1: Tensor network representation of the boundary contractions of Definition 3.4.1. The blue tensors represent those of the original MPS $|v\rangle$, whose physical dimension – the number of physical indices – is d. The rounded red tensor corresponds to the partial isometry, whose free physical index is of dimension B. By blocking these partial isometries $U_v : \mathbb{C}^{d(n-i)} \to \mathbb{C}^B$, these right halves can be boundary contracted, leaving a large tensor of physical dimension B, indicated in green.

By assumption we have avoided the issue of frustration, the second issue surrounding decoupling is the quantum marginal problem (QMP) described in Section 2.4. Whilst a minimum of H most also be a minimum of H_L, the converse is not true. Indeed there exist systems for which the degeneracy in H can be constant, whilst the degeneracy is H_L can be exponentially large; an example of such a system is given in Appendix D.

As a result we cannot necessarily afford to capture a full basis of minima to H_L, especially if its degeneracy grows. An algorithm which does essentially this – and thus cannot be efficiently run for systems such as that described in Appendix D – is studied in Ref. [4]. Instead of attempting to find all potential witnesses however, we need only capture enough states to generate a viable set. As it turns out, we only need a constant number of such states to do this. Central to circumventing the QMP is the concept of *boundary contraction*.

Definition 3.4.1 (Boundary Contraction [1])**.** Given a state of Schmidt rank B and Schmidt decomposition across the $(i, i+1)$ cut given by $|v\rangle = \sum_{j=1}^{B} \lambda_j |a_j\rangle |b_j\rangle$, let $U_v : \mathbb{C}^B \to \mathcal{H}_R$ be the partial isometry specified by $U_v |j\rangle = |b_j\rangle$, abusing notation by writing U_v^* for $I \otimes U_v^*$ when acting on $\mathcal{H}_{[k,n]}$ for $k \leq i+1$.

- Define the left state of $|v\rangle$ be $|\mathrm{ls}(v)\rangle := U_v^* |v\rangle = \sum_j \lambda_j |a_j\rangle |j\rangle \in \mathcal{H}_L \otimes \mathbb{C}^B$.
- Define the boundary contraction of v to be

$$\mathrm{cont}(v) := \mathrm{Tr}_{[1,\cdots,i-1]} \left(|\mathrm{ls}(v)\rangle\langle \mathrm{ls}(v)| \right) = U_v \, \mathrm{Tr}_{[1,\ldots,i-1]} \left(|v\rangle\langle v| \right) U_v^*$$

  Then $\mathrm{cont}(v)$ is a density matrix supported on $\mathcal{H}_i \otimes \mathbb{C}^B$.

Tensor network diagrams of these definitions are given in Figure 3.1.

For a viable set we need only capture the portion of a witness state supported on the first i spins, so we need only find the left state as defined above[4]. As such we can collapse the right half of the chain – spins $i+1$ through n – into one large virtual spin of size B.

The information within a state can be thought of as splitting into three parts now: the left state, the analogous right state, and the boundary contraction that captures the relationship between the two. As the definition of viability only requires the portion of the witness supported on the left half-chain, we don't need the right-state components. The connectedness across the cut however – the boundary contraction – we must concern ourselves with. To compensate for our ignorance we can simply construct a $\xi-net$, also known as a Delone set, in the space of all boundary contractions, and then perform optimisations in the neighbourhood of each net element. Figure 3.2 demonstrates a net on a region of 2D plane, showing what it means for such a net to both be covering and well-spaced.

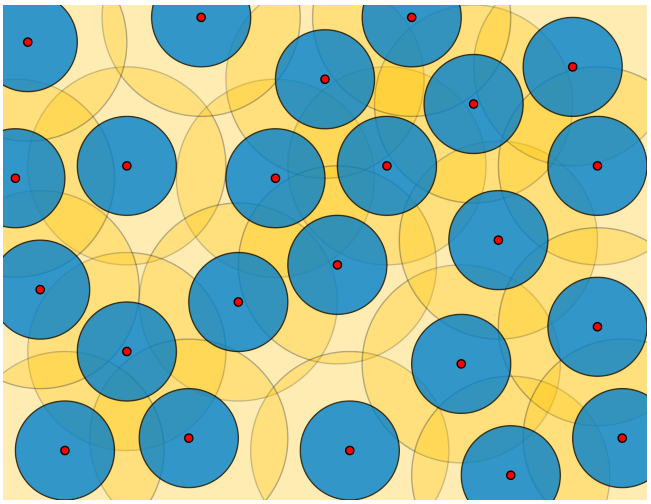


Figure 3.2: [76] The red points constitute a ξ-net. The packing radius ξ here is indicated by the yellow circles. To say that this net has the covering property, as in Lemma 3.4.3, is to say that all points lie in at least one yellow circle, as shown here. The blue circles correspond to a radius half the packing radius, their disjointedness is an indication this net is well-spaced.

Definition 3.4.2 (ξ-net [1])**.** For any integers B, d and $\eta > 0$, a ξ-net on $\mathbb{C}^d \times \mathbb{C}^B$ is given by

$$\mathcal{N}_\xi := \mathcal{I}_\xi^d \times \mathcal{I}_\xi^B \qquad \text{where} \qquad \mathcal{I}_\xi := \left\{-1, -1 + \left\lfloor \xi/B^2d^2 \right\rfloor, \ldots, 1 - \left\lfloor \xi/B^2d^2 \right\rfloor, 1\right\} .$$

The cardinality of such a net is $(2\lceil Bd/\xi \rceil)^{2Bd}$, allowing it to be efficiently handled.

The advantage of using such a net is that any boundary contraction – including that of the actual ground states – is close in trace norm to a net element.

Lemma 3.4.3 (ξ-net covering property [1])**.** *For every $Y \in \mathbb{C}^d \otimes \mathbb{C}^B$ with trace-norm at most 1, there is a $X \in \mathcal{N}_\xi$ such that*

$$\|Y - X\|_1 \leq \xi .$$

It should be noted that whilst the left-Hamiltonian H_L must be optimised in the frustrated case, as the ground energy is known in the frustrated case, this optimisation is unnecessary and the desired states can merely be selected.

Merely being able to find low energy states that are close – in some sense – to a desired witness however is not sufficient to ensure the existence of *two* witnesses. After performing the first optimisation to provide the first witness, we can project away from these solutions, subject to a low energy constraint. By restricting the energy we restrict to states of high ground-space overlap, and by projecting away we ensure that we achieve two witnesses of minimal overlap.

[4] More specifically the $|a_j\rangle$ components, which both the full and left states share.

Algorithm Step 2: Size Trimming

Let $S_i^{(1)}$ be the $(i, ds, b, \Delta = c\epsilon^3)$-viable set constructed by the extension step. For each pair of elements $X_1, X_2 \in \mathcal{N}_{\epsilon/1000}$ of a net over the boundary contractions of bond dimension $B := B_{c\epsilon^3} = 2^{\tilde{\mathcal{O}}(1/\epsilon)}$:

- Firstly pick a σ_1, a density matrix supported on $\mathrm{Span}\left(S_i^{(1)}\right) \otimes \mathbb{C}^B \subseteq \mathcal{H}_L \otimes \mathbb{C}^B$, obeying the *energetic size-trimming* conditions

$$\begin{aligned} \mathrm{Tr}(\sigma_1) = 1, \quad \sigma_1 \geq 0 \\ \left\| \mathrm{Tr}_{[1,i-1]}(\sigma_1) - X_1 \right\|_1 \leq 200\sqrt{c}\epsilon, \\ \mathrm{Tr}(H_L \sigma_1) \leq \sqrt{c}\epsilon \,. \end{aligned} \tag{3.1}$$

  Let $|u_1\rangle = \sum_{j=1}^{B} |u_{1,j}\rangle\,|j\rangle$ be the Schmidt decomposition of the leading eigenvector of the solution σ_1 and add the union of all $\{|u_{1,j}\rangle\}$ to $S_i^{(2,1)}$. If no such state exists, then ignore this net element.

- Secondly take the variable to be σ_2, a density matrix on the same domain, and solve the *orthogonality size-trimming convex program*

$$\begin{aligned} \min \quad & \mathrm{Tr}\left(P_1 \sigma_2\right) \\ \text{where} \quad & P_1 := \sum_j |u_{1,j}\rangle\langle u_{1,j}| \otimes \mathrm{I}_{\mathbb{C}^B} \end{aligned} \tag{3.2}$$

  also subject to the conditions

$$\begin{aligned} \mathrm{Tr}(\sigma_2) = 1, \ \sigma_2 \geq 0, \\ \left\| \mathrm{Tr}_{[1,i-1]}(\sigma_2) - X_2 \right\|_1 \leq 200\sqrt{c}\epsilon, \\ \mathrm{Tr}(H_L \sigma_2) \leq \sqrt{c}\epsilon \,. \end{aligned}$$

  Once again let $|u_2\rangle = \sum_{j=1}^{B} |u_{2,j}\rangle\,|j\rangle$ be the leading eigenvector of the solution σ_2 and add the union of all $\{|u_{2,j}\rangle\}$ to $S_i^{(2,2)}$.

Return the set that combines the solutions to both steps $S_i^{(2)} := S_i^{(2,1)} \cup S_i^{(2,2)}$.

Claim 2 (Proof in Sections 4.3, 4.4, 4.4)**.** *The set $S_i^{(2)}$ is $(i, p_1(n), dsb, \Delta = 1/100)$-viable.*

Size trimming has two downsides. The first is that the bond dimension – the amount of entanglement rank the MPS represents – has grown from b to dsb, and the second is that the error has grown dramatically to $\Delta = 1/100$.

By truncating the MPS representations – that are guaranteed to give a good approximation by the Eckhart-Young Theorem [74] – we can easily reduce the bond dimension with a minimal increase in error. To address the error, we can construct and apply the Hastings' AGSP described in Section 2.5.1 and Appendix B.

3.4.3 Bond Truncation

The idea here is to argue that – due to the area law – there exist low-rank approximate ground states, and thus by truncating a low-energy state in an optimal way, its energy must stay low.

Definition 3.4.4 (Truncation)**.** Given a state $|v\rangle$ with Schmidt decomposition $|v\rangle = \sum_j \lambda_j\,|a_j\rangle\,|b_j\rangle$

across the $(i, i+1)$ cut, and an integer D, then

$$\text{Trunc}_D^i |v\rangle := \sum_{j=1}^{D} \lambda_j |a_j\rangle |b_j\rangle \ .$$

For MPS this manifests as a reduction of the bond dimension. A nice feature of this notion of truncation – thought of as a low-rank approximation – is that it's guaranteed to be optimal.

Lemma 3.4.5 (Eckart-Young theorem [74]). *Let $|v\rangle$ have Schmidt decomposition $|v\rangle = \sum_j \lambda_j |a_j\rangle |b_j\rangle$ across the $(i, i+1)$ cut. For any integer D the trimmed vector $|v'\rangle := \text{Trunc}_D^i |v\rangle / \left\|\text{Trunc}_D^i |v\rangle\right\|$ is an optimal low rank approximation in that $\langle v|v'\rangle \geq |\langle v|w\rangle|$ for any $|w\rangle$ of Schmidt rank at most D across the given cut.*

Next we need to argue that low-rank approximate ground states exist. The state-of-the-art degenerate form of the area law gives the following lemma.

Lemma 3.4.6 (Huang [2]). *For any $c > 0$ there is a constant $C \geq 1$ such that for every n there is a vector $|v\rangle$ with Schmidt rank bounded by $\exp\left(C(\log n)^{3/4}\epsilon^{-1/4}\right)$ across a given cut such that $|\langle\Gamma|v\rangle| \geq 1 - n^{-c}$ for some ground state $|\Gamma\rangle$.*

This is the important corollary of the area law mentioned in Section 2.7. This however is not sufficiently strong; we will require that there exists a full basis of area law states for each cut such that the entire ground space obeys an area law. The specific scaling of the area law we assume doesn't matter; any area law would be sufficient. For simplicity we are going to assume the same scaling as Lemma 3.4.6.

Assumption 3.4.7. *For a two-fold degenerate system, for any $c > 0$ there is a constant $C \geq 1$ such that for every n there is a pair of orthonormal vectors $|v_1\rangle$ and $|v_2\rangle$ with Schmidt rank bounded by $\exp\left(C(\log n)^{3/4}\epsilon^{-1/4}\right)$ across every cut such that $|\langle\Gamma_j|v_j\rangle| \geq 1 - n^{-c}$ for some ground states $|\Gamma_1\rangle$, $|\Gamma_2\rangle$.*

Let $r(n)$ be the polynomial such that there exist an orthonormal pair of states $|v_1\rangle$, $|v_2\rangle$, both with bond dimension $r(n)$, and ground state overlap at least $1 - 1/1000$, which is guaranteed to exist by Lemma 3.4.6/Assumption 3.4.7, with the asymptotics

$$r(n) = 2^{\mathcal{O}(\epsilon^{-1/4}\log^{3/4} n)} = n^{o(1)}$$

Further, define $p_2(n) := 400n\, r(n)$.

Algorithm Step 3: Bond Truncation

Take each vector within $S_i^{(2)}$, and truncate all bonds on $1, \ldots, i-1$ to $p_2(n)$. Return the set $S_i^{(3)}$, comprised of all of these trimmed vectors.

$$S_i^{(3)} := \left\{ \text{Trunc}_{p_2}^1 \text{Trunc}_{p_2}^2 \cdots \text{Trunc}_{p_2}^i |s\rangle \middle| \forall s \in S_i^{(2)} \right\} .$$

Claim 3 (Proof in Section 4.5). *The set $S_i^{(3)}$ is $(i, p_1(n), p_2(n), \delta = 1/4)$-viable.*

A quick recap: at this stage in the algorithm we can show that a viable set on $i-1$ spins can be extended to a i spin viable set. Whilst we have been able to control the number of variables required to describe this set, i.e. the size and bond dimension, the error of this set has grown significantly. Next we want to push this error back down, specifically going from $\delta = 1/4$ to $\Delta = c\epsilon^4$, in an efficient manner.

This leaves only the error that we need to reduce back down to the $\Delta = c\epsilon^3$ at which we started.

3.4.4 Error reduction

The AGSP on which we base our error reduction is the Hastings' AGSP, as developed in the preceding algorithm Ref. [3] and discussed in more detail in Appendix C. The AGSP is given by

$$A := \exp\left[-\frac{xH^2}{2\epsilon^2}\right]$$

where x is a parameter controlling how powerful the AGSP is, i.e. its norm bound orthogonal to the ground space, which is at most $e^{-x/2}$.

This AGSP cannot be directly constructed however, as it would require the exponentiation of H, which would be roughly as difficult as exactly solving for a ground state. One advantage of this AGSP however is that, with the correct parameters, it can be sufficiently well approximated for our purposes. The key to approximating this AGSP is its Fourier transform.

$$A = \frac{\epsilon}{\sqrt{2\pi x}} \int_{-\infty}^{\infty} \exp\left[-\frac{\epsilon t^2}{2x}\right] \exp(-iHt)\,\mathrm{d}t\,.$$

The approximate AGSP[5] we use is given by

$$K := \frac{2\epsilon\tau}{\sqrt{2\pi x}} \sum_{j=0}^{\lceil T/\tau \rceil} \exp\left[-\frac{\epsilon^2\tau^2 j^2}{2x}\right] U_B(\tau j)$$

where $U_B(t)$ is a rank-B approximation of $\exp(-iHt)$, the construction and analysis of which is given in Ref. [77].

This approximation is broken into three distinct approximations. The first is that the integral on $(-\infty, \infty)$ is truncated to an integral on $(-T, T)$, with an exponentially small error in T. The second is that this integral is approximated by a Riemann sum – rectangle rule specifically[6] – with a discrete step-size of τ. The third is that $\exp(-iHt)$ is low-rank approximated by $U_B(t)$. All three errors are considered in Appendix C. If we take parameters with the scaling

$$\begin{aligned} x :=& \mathcal{O}(\log \zeta^{-1}) \\ T :=& \mathcal{O}(\epsilon^{-1} \log \zeta^{-1}) \\ \tau^{-1} :=& \mathcal{O}(n\zeta^{-1}\sqrt{\log \zeta^{-1}}) \\ B :=& (\zeta^{-1})^{\mathcal{O}(1/\epsilon)} \cdot \mathsf{poly}(n/\zeta) \end{aligned}$$

Then this approximate AGSP is capable of lowering the error down to $\Delta = \zeta$, as such we will henceforth refer to this as a ζ-approximate AGSP.

Algorithm Step 4: Error Reduction ($i < n$)

Decompose a $c\epsilon^3$-approximate AGSP as $K = \sum_k A_j \otimes B_j$.
Return the set $S_i^{(4)} := \left\{ A_j \left|s\right\rangle \middle| \forall j,\ \left|s\right\rangle \in S_i^{(3)} \right\}$.

Claim 4 (Proof in Section 4.6)**.** *The set $S_i^{(4)}$ is $(i,\ p(n)\,p_1(n),\ p(n)\,p_2(n),\ \Delta = c\epsilon^3)$-viable set.*

This completes our induction, constructing a $(i, p(n)p_1(n), p(n)p_2(n), \Delta = c\epsilon^3)$-viable set, from a $(i-1, p(n)p_1(n), p(n)p_2(n), \Delta = c\epsilon^3)$-viable set. Moreover this can be done in $n^{\mathcal{O}(1)}$-time.
For the last iteration, $i = n$, the extension, size-trimming and bond truncation steps are unchanged. The error reduction step however is modified, running with with a much stronger $\eta/3$-approximate AGSP.

[5] The double use of approximate (c.f. 'ATM machine') is intentional – albeit clunky – to ensure consistency with previous authors' definitions of AGSPs.

[6] Higher-order approximations such as other Newton-Cotes formulae could be used, though this won't change the overall scaling of the various parameters.

Algorithm Step 4: Error Reduction ($i = n$)

Decompose a $\eta/3$-approximate AGSP as $K = \sum_k A_j \otimes B_j$.
Return the set $S_n^{(4)} := \left\{ A_j \left| s \right\rangle \middle| \forall j,\, \left| s \right\rangle \in S_n^{(3)} \right\}$.

Claim 5 (Proof in Section 4.6)**.** *The set $S_n^{(4)}$ is $(i,\, p_0(n)\, p_1(n),\, p_0(n)\, p_2(n),\, \Delta = \eta/3)$-viable set.*

This is the only step in the entire algorithm to involve p_0 – the dominant parameter – and thus forms a bottleneck for the rest of the algorithm. Indeed the runtime of this step will have the same scaling as p_0, giving an overall runtime of

$$T = (1/\eta)^{\mathcal{O}(1/\epsilon)} \cdot \mathsf{poly}(n/\eta)$$

which reduces to $T = n^{\mathcal{O}(1/\epsilon)}$ for $\eta^{-1} = n^{\mathcal{O}(1)}$ and $T = n^{\mathcal{O}(1)}$ for $\eta^{-1} = n^{o(1)}$, as stated in Theorem 1.

3.4.5 Final Optimisation

As discussed in Section 3.2, once the desired $i = n$, $\Delta \sim \eta$ viable set is constructed, then simply optimising the Hamiltonian on this set yields the final approximate ground states. This set is, by construction, polynomial sized, allowing for this to be done efficiently.

Last Algorithm Step: Final Convex Optimisation

Let $S_n^{(4)}$ be the $(n, \eta/3)$-viable set constructed by the final error reduction.

- Firstly optimise for σ_1, a density matrix supported on Span $\left(S_n^{(4)}\right) \subseteq \mathcal{H}$, as per the program

$$\begin{aligned} \min \quad & \mathrm{Tr}(\sigma_1 H) \\ \text{where} \quad & \sigma_1 \geq 0,\ \ \mathrm{Tr}(\sigma_1) = 1\,. \end{aligned}$$

  Let $|v_1\rangle$ be the MPS representing leading eigenvector of the solution σ_1.

- Secondly optimise for σ_2, a density matrix also supported on Span $\left(S_n^{(4)}\right) \subseteq \mathcal{H}$, as per the program

$$\begin{aligned} \min \quad & \mathrm{Tr}(\sigma_2 H) \\ \text{where} \quad & \langle v_1 | \sigma_2 | v_1 \rangle = 0, \\ & \sigma_1 \geq 0,\ \ \mathrm{Tr}(\sigma_1) = 1 \end{aligned}$$

  Again take $|v_2\rangle$ be the MPS representing leading eigenvector of the solution σ_2.

The MPS vectors $|v_1\rangle$ and $|v_2\rangle$ are the final results of the algorithm.

Claim 6 (Proof in Section 4.7)**.** *The two resulting MPS vectors $|v_1\rangle$ and $|v_2\rangle$ are orthonormal, and ground state overlap at least $1 - \eta$.*

Beware of bugs in the above code; I have only proved it correct, not tried it.
– Donald E. Knuth, *Note to Peter van Emde Boas*

Chapter 4

Proof

In this chapter we will prove all of the viability bounds claimed in the chapter previous.

4.1 Preliminaries

First we need two lemmas about approximately equal states, viz. states with large overlap. The first lemma gives that this sense of approximate equality is transitive, and the second that carries over to approximate equality of expectation values.

Lemma 4.1.1 ([1])**.** *Suppose that* $|\langle w|v\rangle| \geq 1-\delta$ *and* $|\langle w|v'\rangle| \geq 1-\delta'$*, then* $|\langle v|v'\rangle| \geq 1-2(\delta+\delta')$*.*

Lemma 4.1.2 ([3])**.** *For two states of large overlap* $|\langle v|v'\rangle| \geq 1-\delta$ *the difference of expectation values of an operator* O *with* $\|O\| = 1$ *is bounded*

$$\left|\langle v|O|v\rangle - \langle v'|O|v'\rangle\right| \leq 2\sqrt{2\delta}$$

The new feature of the degenerate viable set – as defined in Section 3.1 – is that both witnesses are required to be orthogonal. When performing calculations on viable sets, the two witnesses will tend to become slightly overlapping. To correct this we need to orthogonalise these witnesses, which will in turn tend to slightly raise their energy/lower their ground state overlap.

Lemma 4.1.3 (Orthogonalising Lemma)**.** *Given two low-energy states* $|v_1\rangle$ *and* $|v_2\rangle$ *with overlap at most* $|\langle v_1|v_2\rangle| \leq \omega$*. These two vectors can be orthogonalised into an orthonormal pair* $|v_1'\rangle$*,* $|v_2'\rangle$ *such that the span is left unchanged, and the energy bound grows by* $(1+\omega)/(1-\omega)$*.*

Proof. Define the orthogonalised vectors

$$|v_1'\rangle := |v_1\rangle \qquad\qquad |v_2'\rangle := \frac{|v_2\rangle - |v_1\rangle\langle v_1|v_2\rangle}{\||v_2\rangle - |v_1\rangle\langle v_1|v_2\rangle\|}.$$

Next suppose both states have an energy upper bound of $\langle v_j|H|v_j\rangle \leq \Delta$. The energy of the first state is clearly unchanged – as for the second, expanding the definition gives

$$\begin{aligned}\langle v_2'|H|v_2'\rangle &= \left[\frac{\langle v_2| - \langle v_2|v_1\rangle\langle v_1|}{\|\langle v_2| - \langle v_2|v_1\rangle\langle v_1|\|}\right] H \left[\frac{|v_2\rangle - |v_1\rangle\langle v_1|v_2\rangle}{\||v_2\rangle - |v_1\rangle\langle v_1|v_2\rangle\|}\right] \\ &= \frac{\langle v_2|H|v_2\rangle - 2\,\mathrm{Re}\left[\langle v_2|v_1\rangle\langle v_1|H|v_2\rangle\right] + |\langle v_1|v_2\rangle|^2\langle v_1|H|v_1\rangle}{1-|\langle v_1|v_2\rangle|^2}.\end{aligned}$$

As for the cross term $\langle v_1|H|v_2\rangle$, we can use the positivity of H and the Cauchy-Schwarz inequality to give that it is bounded by the geometric mean of the two energies

$$\begin{aligned}|\langle v_1|H|v_2\rangle| &= \left|\langle v_1|\sqrt{H}\sqrt{H}\,|v_2\rangle\right| \\ &\leq \left\|\langle v_1|\sqrt{H}\right\|\left\|\sqrt{H}\,|v_2\rangle\right\| \\ &= \sqrt{\langle v_1|H|v_1\rangle}\sqrt{\langle v_2|H|v_2\rangle}\end{aligned}$$

which in turn allows us to bound the energy of $|v_2'\rangle$

$$\begin{aligned}\langle v_2'|H|v_2'\rangle &\leq \frac{\langle v_2|H|v_2\rangle + 2\,|\langle v_1|v_2\rangle|\,\sqrt{\langle v_1|H|v_1\rangle}\sqrt{\langle v_2|H|v_2\rangle} + |\langle v_1|v_2\rangle|^2\,\langle v_1|H|v_1\rangle}{1-|\langle v_1|v_2\rangle|^2} \\ &= \frac{\left[\sqrt{\langle v_2|H|v_2\rangle} + |\langle v_1|v_2\rangle|\,\sqrt{\langle v_1|H|v_1\rangle}\right]^2}{1-|\langle v_1|v_2\rangle|^2} \\ &\leq \frac{[E+\omega E]^2}{1-\omega^2} = \frac{1+\omega}{1-\omega}\,E\,.\end{aligned}$$

By replacing H with the projector complementary to the ground space, the same growth factor can be shown to hold for the ground state overlap. □

4.1.1 Low-entanglement approximate ground states

In this subsection we will lay out the lemmas surrounding the area law. First we consider a set of low-rank approximate ground states given by truncation, and then argue that truncating other approximate ground state doesn't blow their error up too much as a consequence.

Lemma 4.1.4 ([2],[3])**.** *Given a ground state $|\Gamma\rangle$, then the low-rank truncation across cut $(i, i+1)$ given by*

$$|v\rangle := \mathrm{Trunc}^i_{B_\delta}|\Gamma\rangle \,/\, \left\|\mathrm{Trunc}^i_{B_\delta}|\Gamma\rangle\right\| \qquad \textit{where} \qquad B_\delta := \exp\left(\tilde{\mathcal{O}}(\epsilon^{-1}+\epsilon^{-1/4}\log^{3/4}\delta^{-1})\right)$$

has ground state overlap $|\langle\Gamma|v\rangle| \geq 1-\delta$.

Given state-of-the-art results of Ref. [2] this result holds for one ground state across every given cut. The extended area law of Assumption 3.4.7 extends this to all ground states, allowing them all to be efficiently represented [75]. Next we need that the truncation doesn't blow up the energy of an approximate ground state.

Lemma 4.1.5 ([1])**.** *Suppose we have a state $|w\rangle$ with $\langle w|H|w\rangle \leq \Delta\epsilon$ with $\Delta \leq 1/4(1+\epsilon)$, then $\langle v|H|v\rangle \leq 48\sqrt{\Delta}$ where $|v\rangle := \mathrm{Trunc}_{B_{\Delta\epsilon}}|w\rangle \,/\, \|\mathrm{Trunc}_{B_{\Delta\epsilon}}|w\rangle\|$.*

Combining these we can get the existence low-rank approximate ground states, both in terms of overlap *and* energy.

Corollary 4.1.6. *Across any given cut – for a δ such that $\delta(1+1/\epsilon) \leq 1/3$ – there exists an orthonormal pair of approximate ground states of entanglement rank B_δ with energy at most $48\sqrt{\delta}$ and ground state overlap at least $1-\delta$.*

Proof. Following the proof in [3] – Lemma 6 specifically – we obtain an energy bound of $24\sqrt{\delta}$ and ground space overlap bound of $1-\delta/2$. In this proof it was shown that the difference between the original states and their truncations has a norm at most $\sqrt{\delta(1+1/\epsilon)}$. As a result if we start with a pair of orthogonal ground states – with overlap 0 – the truncation results in an overlap at most $\delta(1+1/\epsilon) \leq 1/3$. Applying the orthogonalisation of Lemma 4.1.3 these bounds worsen by a factor of at most 2, giving the desired results. □

With these preliminary lemmas we can now start the proofs.

4.2 Extension

The extension procedure is in fact quite trivial, the proof not requiring any of the above lemmas.

Proof of Claim 1 The result of Algorithm Step 1, $S_i^{(1)}$, is $(i, ds, b, \Delta = c\epsilon^3)$-viable

Proof. As $\{|j\rangle\}$ span $\mathcal{H}_i$ we have that $\mathrm{Span}\left(S_i^{(1)}\right) = \mathrm{Span}\left(S_{i-1}\right) \otimes \mathcal{H}_i$ and the newly constructed set inherits the existing witnesses. As such the set is extended to the next spin at the cost of a multiplicative growth in the cardinality. □

4.3 Size Trimming

Next is the size-trimming procedure; this is by far the least trivial step to prove. In this section we will set forth the lemmas and facts needed for both size-trimming procedures. The proof of each procedure is given in the next two sections. The lemmas we need come in two groups: firstly those pertaining to boundary contraction, and secondly those concerning the existence of low-energy states.

4.3.1 Boundary contraction

First we need to lay out a lemma used for boundary contraction. Divide the Hamiltonian up into three parts across the $(i, i+1)$ cut, $H_L = H_1 + \cdots + H_{i-1}$, H_i, and $H_R := H_{i+1} + \cdots + H_{n-1}$. We now want to argue that the energy of a reduced density operator is bounded by its left-energy and how close its boundary contraction is to a given approximate ground state; this is the *decoupling* mentioned in Section 2.4.

Lemma 4.3.1 ([1, 3])**.** *Let σ be a density matrix on $\mathcal{H}_{[1,i]} \otimes \mathbb{C}^B$ and $|v\rangle = \sum_{j=1}^{B} \lambda_j |a_j\rangle |b_j\rangle \in \mathcal{H}$ be a Schmidt-decomposed state. The density matrix $\sigma' := U_v \sigma U_v^\dagger$ on $\mathcal{H}$ satisfies*

$$\begin{aligned}\mathrm{Tr}\left(\sigma' H\right) \leq \mathrm{Tr}(\sigma H_L) + \langle v|(H_i + H_R)|v\rangle \\ + \left\|\mathrm{Tr}_{[1,i-1]}\left(\sigma\right) - \mathrm{cont}(v)\right\|_1 \cdot \left(1 + \max_{|b\rangle \in \mathrm{Span}\{|b_j\rangle\}} \langle b|H_R|b\rangle\right).\end{aligned}$$

4.3.2 Low-energy states

To bound the right hand term in the above lemma, we need the truncation lemma [2, 67, 3]. In essence this says that a low-energy state can be well approximated by locally low-energy terms. For an unfrustrated system however this lemma is trivial; a ground state minimises every local Hamiltonian term.

Definition 4.3.2. Define $\mathcal{H}_{[i,j]}$ to be the Hilbert space on spins i through j. Denote by $\mathcal{G}_{[i,j]}$ the subset of this Hilbert space which also minimises the respective Hamiltonian terms.

In this notation the truncation lemma can be expressed as:

Lemma 4.3.3 (Unfrustrated truncation lemma)**.** *For any ground state $|\Gamma\rangle$, the reduced density operator $\sigma_{[i,j]}$ on $[i,j]$ is supported entirely on $\mathcal{G}_{[i,j]}$.*

Next we need to argue the existence of low-energy states that our size-trimming procedures are selecting from. These two low-energy states are taken by extending the existing witnesses.

Lemma 4.3.4. *There exist an orthonormal pair of states $\{|w_j\rangle\} \subseteq \mathrm{Span}\left(S_i^{(1)}\right) \otimes \mathcal{G}_{[i+1,n]}$ with bond dimension $B_{c\epsilon^3}$, with energy $\langle w_j|H|w_j\rangle \leq 100\sqrt{c}\epsilon$.*

Proof. Take $\{\left|v_j'\right\rangle\}$ to be the witnesses of the existing $(i, \Delta = c\epsilon^3)$-viable set, such that $\left\langle v_j'\right|H\left|v_j'\right\rangle \leq c\epsilon^3$. Applying Lemma 4.1.5 we get that the trimmed states $|v_j\rangle := \mathrm{Trunc}_{B_{c\epsilon^3}}\left|v_j'\right\rangle / \left\|\mathrm{Trunc}_{B_{c\epsilon^3}}\left|v_j'\right\rangle\right\|$ have

$$\langle v_j|H|v_j\rangle \leq 48\sqrt{c}\epsilon\,.$$

Take an orthonormal pair of states $|u_j\rangle$ with $\langle u_j|\Gamma_j\rangle \geq 1 - c\epsilon^3$ and bond dimension $B_{c\epsilon^3}$, whose existence is guaranteed by Corollary 4.1.6. Applying Lemma 4.1.1 gives $\left|\left\langle u_j\right|v_j'\right\rangle\right| \geq 1 - 4c\epsilon^3$, and

using this to in turn bound the overlap of $\{|v_j\rangle\}$ gives

$$\begin{aligned}
|\langle v_1|v_2\rangle| &= \Big| \langle v_1|u_1\rangle \langle u_1|v_2\rangle + \langle v_1|u_2\rangle \langle u_2|v_2\rangle \\
&\qquad + \langle v_1|(I - |u_1\rangle\langle u_1| - |u_2\rangle\langle u_2|)|v_2\rangle \Big| \\
&\leq |\langle v_1|u_1\rangle \langle u_1|v_2\rangle| + |\langle v_1|u_2\rangle \langle u_2|v_2\rangle| \\
&\qquad + |\langle v_1|(I - |u_1\rangle\langle u_1| - |u_2\rangle\langle u_2|)|v_2\rangle| \\
&\leq 12\sqrt{2c\epsilon^3\,(1 - 2c\epsilon^3)} \\
&\leq 12\sqrt{2c\epsilon^3}\,.
\end{aligned}$$

Imposing $12\sqrt{2c\epsilon^3} \leq 1/3$ – which holds for $\epsilon \leq 3000$ and $c = 10^{-14}$ – the orthogonalisation procedure of Lemma 4.1.3 increases the energy by at most a factor of 2, and thus orthogonalising $\{|v_j\rangle\}$ gives orthonormal states of energy at most $96\sqrt{c}\epsilon$. Take P to be the projector onto $\mathcal{H}_{[1,i]} \otimes \mathcal{G}_{[i+1,n]}$. The projection of our two states down onto that space – $|w_i\rangle := P\,|v_i\rangle \,/\, \|P\,|w_i\rangle\|$ – have overlap

$$\begin{aligned}
|\langle w_1|w_2\rangle| &\leq \frac{\langle v_1|P|v_2\rangle}{\|\langle v_1|\,P\| \cdot \|P\,|v_2\rangle\|} \\
&\leq \frac{2 \cdot 96\sqrt{c}}{(1 - 96\sqrt{c})^2} \\
&\leq 2 \times 10^{-5} \leq 1/49\,.
\end{aligned}$$

Applying the orthogonalisation of Lemma 4.1.3 in turn increases the energy by a factor of 100/96, raising the energy bound to the $100\sqrt{c}\epsilon$ stated. □

This proves the existence of low-energy states, a necessity for the size trimming. We next want to argue that any such low-energy states necessarily have a large overlap with these w states.

Lemma 4.3.5. *Any vector $|w\rangle \in \mathrm{Span}\{|w_1\rangle, |w_2\rangle\}$ has energy at most $200\sqrt{c}\epsilon$. Furthermore any vector $|v\rangle$ with energy at most $\Delta\epsilon$ has overlap with this w-space at least $1 - 2\,(\Delta + 20\sqrt{c})$.*

Proof. Take a vector $|w\rangle = \lambda\,|w_1\rangle + \sqrt{1-\lambda^2}\,|w_2\rangle$ then

$$\begin{aligned}
\langle w|H|w\rangle &= \lambda^2\,\langle w_1|H|w_1\rangle + 2\lambda\sqrt{1-\lambda^2}\,\mathrm{Re}\,[\langle w_1|H|w_2\rangle] + \left(1-\lambda^2\right)\langle w_2|H|w_2\rangle \\
&\leq \left(\lambda\sqrt{\langle w_1|H|w_1\rangle} + \sqrt{1-\lambda^2}\sqrt{\langle w_2|H|w_2\rangle}\right)^2 \\
&\leq \left(\lambda + \sqrt{1-\lambda^2}\right)^2 100\sqrt{c}\epsilon \\
&\leq 200\sqrt{c}\epsilon\,.
\end{aligned}$$

By Lemma 3.1.2 to a state of energy at most $\Delta\epsilon$, then applying Lemma 4.1.1 to the resulting ground state overlap, such a state can be shown to overlap with the w-space the desired $1 - 2\Delta - 400\sqrt{c}$. □

Now we want to prove the existence of the desired witnesses.

4.4 Energetic Size Trimming

Denote σ_1 to be the solutions of *energetic size trimming* for X_1 closest to $\mathrm{cont}(w_1)$ (see Figure 3.2), and $|u_1\rangle$ the leading eigenvectors.

Lemma 4.4.1 (Energetic Solution)**.** *For $|u_1\rangle = \sum_j |u_{1,j}\rangle\,|j\rangle$ there exist an orthonormal basis $\{r_j\} \subseteq \mathcal{G}_{[i+1,n]}$, such that $|u_1'\rangle := \sum_j |u_{1,j}\rangle\,|r_j\rangle$ has energy at most $1200\sqrt{c}\epsilon$.*

Proof. Firstly take $\sigma_1' := U_{w_1}\sigma_1 U_{w_1}^\dagger$ and applying 4.3.1 and using the convex conditions of Equation (3.1) we have

$$\begin{aligned}\mathrm{Tr}\left(\sigma_1' H\right) &\leq \mathrm{Tr}\left(\sigma H_L\right) + \langle w_1|(H_i + H_R)|w_1\rangle \\ &\quad + \left\|\mathrm{Tr}_{[1,i-1]}(\sigma_1) - \mathrm{cont}(w_1)\right\|_1 \cdot \left(1 + \max_j \langle r_{1,j}|H_R|r_{1,j}\rangle\right) \\ &\leq \langle w_1|H|w_1\rangle + \left\|\mathrm{Tr}_{[1,i-1]}(\sigma_1) - \mathrm{cont}(w_1)\right\|_1 \\ &\leq 400\sqrt{c}\epsilon\,.\end{aligned}$$

Next eigendecompose this density matrix $\sigma_1' = \sum_k \lambda_k |v_k\rangle\langle v_k|$ with λ_k positive and non-increasing. Take K to be the set of indices k for which $\langle v_k|H|v_k\rangle \leq 1200\sqrt{c}\epsilon$. The $|v_k\rangle$ corresponding to $k \in K$ must have an overlap much larger than $1/\sqrt{2}$ with the ground space by Lemma 3.1.2. As the ground space is only two-dimensional it turns out that this overlap only allows for two such vectors, and as such $|K| \leq 2$. This – together with the energy bound $\sum_{k\in K}\lambda_k^2 \geq 2/3$ – gives that the leading eigenvector must correspond to an index in K, and thus be of energy at most $1200\sqrt{c}\epsilon$. □

Orthogonality Size Trimming

As for the second witness the argument must be split. Firstly we will describe a quantity called *left-distinguishability* that encapsulates why the argument must be split. After this we will give the proofs of the viability bounds for both high and low values of this unknown quantity.

4.4.1 Left-distinguishability

Any two states that are orthogonal, may or may not have orthogonal reduced density operators. An example of this are the three qubit[1] states $|\psi_1\rangle = |000\rangle$ and $|\psi_2\rangle = |010\rangle$. The reduced density operators on the first qubit are identical, on the first two qubits however they are orthogonal. In this sense we can say that these two states are entirely *indistinguishable* on the first qubit, whilst they are entirely *distinguishable* on the first two qubits.

If on the domain on which we are performing size trimming – spins 1 through i – the two witnesses are entirely indistinguishable, then the energetic size trimming is sufficient; any viable set for the first witness is also a viable set for the second. If however the two witness are highly distinguishable, then this first procedure is not guaranteed to give a good second witness, so we need to project away from the existing vectors. This is the idea behind the orthgonality size-trimming procedure. As such we want to quantify the degree to which our witnesses can be distinguished, and split the argument accordingly.

The measure of left-distinguishability we will use is

$$D := 1 - \sum_j \left\langle u_{1,j}\middle|\mathrm{Tr}_{[i,n]}\left(|w\rangle\langle w|\right)\middle|u_{1,j}\right\rangle$$

where $|w\rangle$ is a member of $\mathrm{Span}(|w_1\rangle, |w_2\rangle)$ perpendicular to $|u_1'\rangle$. If the left vectors span identical spaces then $D = 0$, if they span orthogonal spaces $D = 1$. By considering both low D and high D bounds we can prove viability bounds on $S_i^{(2)}$ independent of this unknown. First we will show this combined proof, before proving the separate bounds.

Proof of Claim 2 The result of Algorithm Step 2, $S_i^{(2)}$, is $(i, p_1(n), dsb, \Delta = 1/100)$-viable.

Proof. The size-trimming bound of $p_1(n)$ comes, to leading order, from the size of the boundary-contraction net as shown in Lemma 3.4.3. The growth of the bond dimension from $b \to dsb$ is the worst-case result considering all the linear combinations necessary. As we will show in Corollaries

[1] Qubit just means a two-state quantum system; see Ref. [78] for more details.

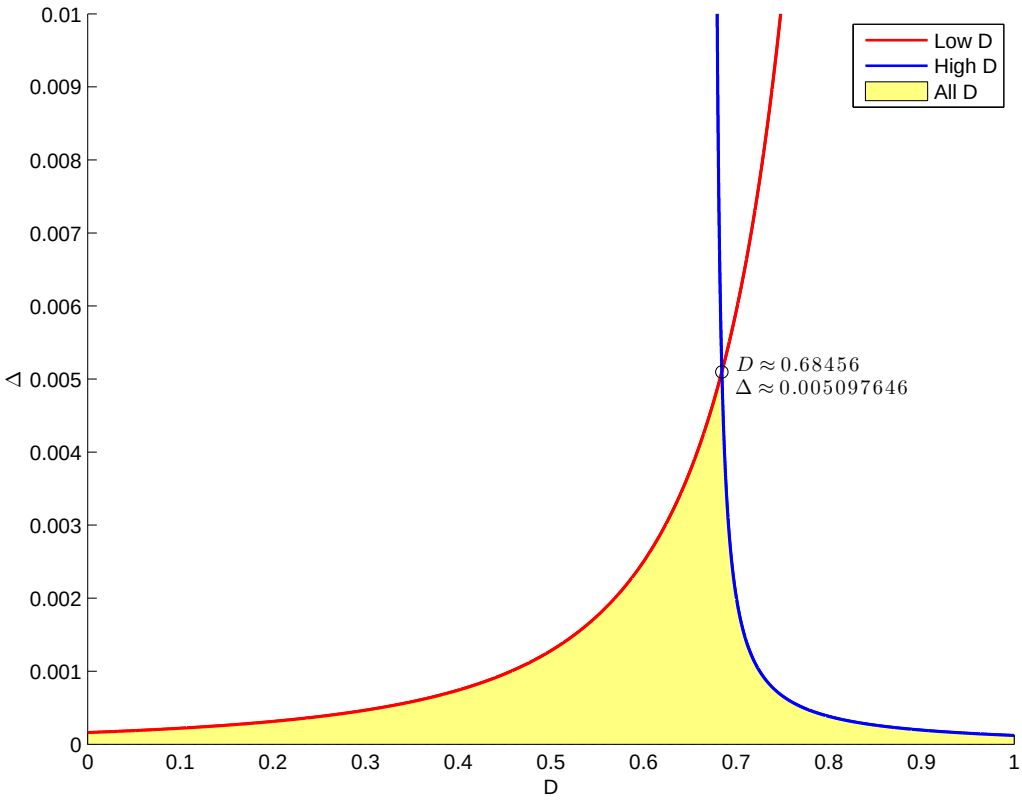


Figure 4.1: Size Trimming Error Levels

4.4.3 and 4.4.7 the low D and high D limits on Δ are

$$\Delta_{\text{Low}} \leq \frac{1600\sqrt{c}}{(1-D)^3}$$

$$\Delta_{\text{High}} \leq 1200\sqrt{c} \cdot \frac{(1-0.2^2)\sqrt{D} + \sqrt{2\sqrt{1-D}\left(\sqrt{1-D}+0.2\right)}}{(1+0.2^2)\sqrt{D} - \sqrt{2\sqrt{1-D}\left(\sqrt{1-D}+0.2\right)}},$$

and so $\Delta \leq \min\{\Delta_{\text{Low}}, \Delta_{\text{High}}\}$. The region bounded by both is shown in Figure 4.1. The intersection occurs at $D \approx 0.6846$, $\Delta \approx 0.005098$, and as such we can conclude – *for any* D – that the overall error is bounded by

$$\Delta < 1/100\,.$$

□

Next we want to prove the above low and high D bounds on Δ.

4.4.2 Low D – Energetic Size Trimming

As stated before, if the two states are indistinguishable – low D – we should expect that the energetic procedure captured both witnesses, viz. there should exist a second witness with left Schmidt vectors in the span of $|u_{1,j}\rangle$. As we need only capture the left Schmidt vectors to ensure viability, this will mean no extra steps are required to capture this second witness.

Lemma 4.4.2 (Low D Solution)**.** *There exist orthonormal basis* $\{|l_j\rangle\} \in \text{Span}\{|u_{1,j}\rangle\}$ *and* $\{|r_j\rangle\} \subseteq \mathcal{H}_{[i+1,n]}$ *such that* $|v\rangle = \sum_j |l_j\rangle\,|r_j\rangle$ *has energy at most* $400\sqrt{c}\epsilon/(1-D)$ *and bounded overlap* $|\langle u_1'|v\rangle| \leq \sqrt{D(2-D)}$.

Proof. Define the projection into Hilbert space of states whose left Schmidt vectors $\{u_{1,j}\}$ – which have already been found – as

$$P := \left(\sum_j |u_{1,j}\rangle\langle u_{1,j}| \right) \otimes I$$

where the identity I either acts on $\mathcal{H}_{[i+1,n]}$ or the boundary contraction $\mathbb{C}^B$, depending on the context. By definition any state in the image of P can therefore be a witness of $\{u_{1,j}\}$. In terms of this projector the distinguishability parameter becomes

$$\mathrm{Tr}\left(P\,|w\rangle\langle w| \right) = \langle w|P|w\rangle = 1 - D\,.$$

Taking $|v\rangle$ to be the closest vector in the image of P to w – specifically $|v\rangle = P\,|w\rangle \,/\, \|P\,|w\rangle\|$ – then this energy bound grows as

$$\langle v|H|v\rangle = \frac{\langle w|H|w\rangle}{\|P\,|w\rangle\|^2} \leq \frac{200\sqrt{c}\epsilon}{1-D}\,.$$

As for the overlap, using the fact that $|u_1'\rangle$ is perpendicular to $|w\rangle$, we have that

$$\left|\langle u_1'|v\rangle\right| \leq \sqrt{D(2-D)}\,.$$

□

This then gives us our viability condition for low D.

Corollary 4.4.3 (Low D viability)**.** *For the viability claim Claim 2, the energetic error Δ is bounded*

$$\Delta \leq 1600\sqrt{c}/\left(1-D\right)^3\,.$$

Proof. By orthogonalising both $|u_1'\rangle$ and $|v\rangle$ as given above, Lemma 4.1.3 gives witnesses with energy bounds

$$\Delta \leq \frac{1+\sqrt{D(2-D)}}{1-\sqrt{D(2-D)}} \cdot \frac{200\sqrt{c}}{1-D} \leq \frac{1600\sqrt{c}}{(1-D)^3}\,.$$

□

4.4.3 High D – Orthogonality Size Trimming

Now we need to argue in the highly distinguishable case; this is where the orthogonality size-trimming comes in.

Take $|u_2\rangle$ to be the solution for the orthogonality size-trimming, with X_2 closest to $\mathrm{cont}(w)$, and $|u_2'\rangle := U_w\,|u_2\rangle$. Decompose this as

$$\left|u_2'\right\rangle = \alpha\,|w\rangle + \beta\left|u_1'\right\rangle + \gamma\,|v\rangle$$

where $|v\rangle$ is perpendicular to both $|w\rangle$ and $|u_1'\rangle$. For simplicity take all three coefficients to be positive; this can be done without loss of generality by absorbing the phases into the states. Then α indicates the overlap with the desired second witness, and we want to argue that this is large. Here β is the overlap with the existing witness, and it will contribute to the orthogonalising error. Finally, γ corresponds to contributions orthogonal to both; these are higher-energy states.

The basic procedure is to project away from the existing left Schmidt vectors – and thus $|u_1'\rangle$ – whilst keeping the energy low. The low energy condition keeps γ from growing, and the projection will shrink β, giving the desired large α; this is the orthogonality size trimming of Section 3.4.2.

By an argument identical to that for $|u_1'\rangle$ as in Lemma 4.4.1, the energy of $|u_2'\rangle$ can be upper bounded by $1200\sqrt{c}\epsilon$ if we take X_2 closest to $\mathrm{cont}(w)$. As for the excited component γ, we have the following bound.

Lemma 4.4.4.

$$\gamma \leq 1/50\,.$$

Proof. First we note that both $|w\rangle$ and $|u_1'\rangle$ have energies below $1200\sqrt{c}\epsilon$. As $|v\rangle$ is perpendicular to both, and as the ground space is two-dimensional, this gives that the energy of $|v\rangle$ must exceed $(1-2400\sqrt{c})\epsilon$. Using the energy bounds on $|u_2'\rangle$ and $|v\rangle$ we have that

$$\begin{aligned}
1200\sqrt{c}\epsilon &\geq \langle u_2'|H|u_2'\rangle \\
&\geq \alpha^2 \langle w|H|w\rangle + 2\,\mathrm{Re}\,\alpha\beta \langle w|H|u_1'\rangle + 2\,\mathrm{Re}\,\alpha\gamma \langle w|H|v\rangle \\
&\quad + \beta^2 \langle u_1'|H|u_1'\rangle + 2\,\mathrm{Re}\,\beta\gamma \langle u_1|H|v\rangle + \gamma^2 \langle v|H|v\rangle \\
&\geq \gamma^2 \langle v|H|v\rangle \\
&= \gamma^2 \epsilon \left(1 - 2400\sqrt{c}\right)\,.
\end{aligned}$$

Inserting the value $c := 10^{-14}$ gives

$$\gamma \leq \sqrt{\frac{3}{24994}} \leq \frac{1}{50}\,.$$

□

Whilst the optimised value of Program 3.2 is unknown, $|w\rangle\langle w|$ serves as a witness of this optimisation; the optimised value is upper bounded by it. By the optimiality of σ_2 we can thus conclude that

$$\begin{aligned}
\mathrm{Tr}\,(\sigma_2 P) &\leq \mathrm{Tr}\left(|w\rangle\langle w|\,P\right) \\
&= \langle w|P|w\rangle \\
&= \sum_j \langle u_{1,j}|\mathrm{Tr}_{[i,n]}\left(|w\rangle\langle w|\right)|u_{1,j}\rangle \\
&=: 1 - D
\end{aligned}$$

and so the smallness of the returned value of the optimisation corresponds to how distinguishable the witnesses were. This gives that the expectation value of P is low for σ_2, and so we should expect that it is also low – though not quite *as* low – for $|u_2\rangle$, the leading eigenvector. Using an argument similar to that of the energy we have:

Lemma 4.4.5.

$$\langle u_2'|P|u_2'\rangle = \langle u_2|P|u_2\rangle \leq 3(1-D)\,.$$

Proof. The first equality is taken from the fact that P only acts non-trivially to the left of the cut whilst U_w is both unitary and trivial to the left (see Figure 3.1).

As for the second inequality we can use the eigenvalue argument used in Lemma 4.4.1. Eigendecompose $\sigma_2 = \sum_k \lambda_k^2 |v_k\rangle\langle v_k|$, where $\sum_k \lambda_k^2 = 1$, $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_B \geq 0$ and $|v_1\rangle =: |u_2\rangle$. As in 4.4.1 we've shown that $\lambda_1^2 + \lambda_2^2 \geq 2/3$ and thus that $\lambda_1^2 \geq 1/3$. The expectation value of P on σ_2 takes the form

$$1 - D \geq \mathrm{Tr}(\sigma_2 P) = \sum_k \lambda_k^2 \langle v_k|P|v_k\rangle$$

and so giving the dominance of the first eigenvalue we have

$$\begin{aligned}
\langle u_2|P|u_2\rangle &= \langle v_1|P|v_1\rangle \\
&\leq \frac{1 - D - \sum_{k=2}^{B} \lambda_k^2 \langle v_k|P|v_k\rangle}{\lambda_1^2} \\
&\leq \frac{1-D}{\lambda_1^2} \\
&\leq 3\,(1-D)\,.
\end{aligned}$$

□

As such we can see this bound is entirely trivial for $D \leq 2/3$. Above this however the bound becomes non-trivial and – together with the bound on γ – allows β to be bounded as well, allowing $|u_1'\rangle$ and $|u_2'\rangle$ to be orthogonalised and the resulting energy bounded.

Lemma 4.4.6 (High D Solution)**.**

$$\beta^2 \leq \frac{2\sqrt{1-D}}{D} \cdot \left(\sqrt{1-D} + \gamma\right) - \gamma^2 .$$

Proof. Using the bounds of the above lemma and simply expanding the decomposition of $|u_2'\rangle$ we have

$$\begin{aligned} 3(1-D) &\geq \langle u_2' | P | u_2' \rangle \\ &\geq \alpha^2 \langle w|P|w\rangle + 2\,\mathrm{Re}\ \alpha\beta \langle w|P|u_1'\rangle + 2\,\mathrm{Re}\ \alpha\gamma \langle w|P|v\rangle \\ &\quad + \beta^2 \langle u_1'|P|u_1'\rangle + 2\,\mathrm{Re}\ \beta\gamma \langle u_1'|P|v\rangle + \gamma^2 \langle v|P|v\rangle \ . \end{aligned}$$

Dropping both β cross-terms we find

$$\begin{aligned} &\geq \alpha^2 \langle w|P|w\rangle + 2\,\mathrm{Re}\ \alpha\gamma \langle w|P|v\rangle + \beta^2 + \gamma^2 \langle v|P|v\rangle \\ &\geq \alpha^2 \langle w|P|w\rangle - 2\alpha\gamma\, |\langle w|P|v\rangle| + \gamma^2 \langle v|P|v\rangle + \beta^2 . \end{aligned}$$

Then using the previously mentioned trick to split $\langle w|P|v\rangle$ into expections,

$$\begin{aligned} &\geq \alpha^2 \langle w|P|w\rangle - 2\alpha\gamma \sqrt{\langle w|P|w\rangle}\sqrt{\langle v|P|v\rangle} + \gamma^2 \langle v|P|v\rangle + \beta^2 \\ &\geq \left(\alpha\sqrt{\langle w|P|w\rangle} - \gamma\sqrt{\langle v|P|v\rangle}\right)^2 + \beta^2 \\ &\geq \left(\alpha\sqrt{1-D} - \gamma\right)^2 + \beta^2 \\ &\geq \alpha^2(1-D) - 2\alpha\gamma\sqrt{1-D} + \beta^2 + \gamma^2 . \end{aligned}$$

Finally, throwing away the last few terms, and using the fact that $\alpha^2 + \beta^2 + \gamma^2 = 1$, we get

$$\begin{aligned} &\geq 1 - D\alpha^2 - 2\alpha\gamma\sqrt{1-D} \\ &\geq 1 - D + D\beta^2 + D\gamma^2 - 2\gamma\sqrt{1-\beta^2-\gamma^2}\sqrt{1-D} \\ &\geq 1 - D + D\beta^2 + D\gamma^2 - 2\gamma\sqrt{1-D} . \end{aligned}$$

Rearranging this gives the desired bound on β. □

Corollary 4.4.7 (High D viability)**.** *For the viability claim Claim 2, the energetic error Δ is bounded*

$$\Delta \leq 1200\sqrt{c} \cdot \frac{1+\beta}{1-\beta}$$

where β is upper bounded as above.

Proof. For this we can simply use the above energy bounds, and apply Lemma 4.1.3 for witness overlap $|\langle u_1'|u_2'\rangle| \leq \beta$. □

4.5 Bond Truncation

The idea here is to use the existence of low-rank approximate ground states, and argue that truncation therefore cannot induce much error. A truncated vector will tend to have large overlap with the original vector:

Lemma 4.5.1 ([1])**.** *Given a vector $|v\rangle$ with Schmidt rank R across the $(i, i+1)$ cut, for any $|u\rangle$*

$$\left|\left\langle \mathrm{Trunc}^i_{R/\delta}(u) \middle| v \right\rangle\right| \geq |\langle u|v\rangle| - \delta .$$

Next, take $|v_1\rangle$ and $|v_2\rangle$ to be the truncations of $|u_1\rangle$ and $|u_2\rangle$ respectively. We should expect large overlap between the truncated and un-truncated witnesses:

Lemma 4.5.2.

$$|\langle v_j|u_j\rangle| \geq 1 - 1/20\,.$$

Proof. Take $|\Gamma_1\rangle$, $|\Gamma_2\rangle$ to be an orthonormal basis for the ground space. For simplicity take $|\Gamma_1\rangle$ to be the closest possible ground state to $|u_1\rangle$, such that it is the ground state projection of $|u_1\rangle$. Decomposing the witness states then

$$\begin{aligned}
|u_1\rangle &= \nu_1 |\Gamma_1\rangle + \sqrt{1-\nu_1^2}\left|\Gamma_1^\perp\right\rangle \\
|u_2\rangle &= \nu_2\left[\mu|\Gamma_2\rangle + \sqrt{1-\mu^2}|\Gamma_1\rangle\right] + \sqrt{1-\nu_2^2}\left|\Gamma_2^\perp\right\rangle
\end{aligned}$$

where $\left|\gamma_1^\perp\right\rangle$ and $\left|\gamma_2^\perp\right\rangle$ are orthogonal to the ground space, and thus have energies at least ϵ, the spectral gap. Using Lemma 3.1.2, the energy bounds turn into ground state overlap bounds $\nu_1, \nu_2 \geq 99/100$, and the orthogonality gives $\mu \geq 999/1000$. This in turn gives that $|\langle u_j|\Gamma_j\rangle| \geq 1 - 1/50$ for both $j = 1, 2$. Similar analysis gives that $|\langle v_j|\Gamma_j\rangle| \geq 1 - 1/500$. Combining these and using Lemma 4.1.1 gives the desired result. □

Proof of Claim 3 The set $S_i^{(3)}$ is a $(i, p_1(n), p_2(n), \delta = 1/4)$-viable set.

Proof. Take $|w_j\rangle$ to be the truncated form of $|u_j\rangle$. As $i \leq n$ truncations are done, each truncated to a bond dimension $400nr(n)$, we can use Lemma 4.5.1 to get

$$|\langle v_j|w_j\rangle| \geq |\langle v_j|u_j\rangle| - n/400n \geq 1 - 1/19$$

Next we need to orthogonalise. The overlap of the truncated states can be bounded using the triangle inequality and ground state overlaps

$$\begin{aligned}
|\langle w_1|w_2\rangle| &= \left|\langle w_1|\Gamma_1\rangle\langle\Gamma_1|w_2\rangle + \left\langle w_1\right|\left(I - |\Gamma_1\rangle\langle\Gamma_1|\right)\left|w_2\right\rangle\right| \\
&\leq |\langle w_1|\Gamma_1\rangle| \cdot |\langle\Gamma_1|w_2\rangle| + |\langle w_1|\Gamma_2\rangle| \cdot |\langle\Gamma_2|w_2\rangle| \\
&\quad + \left|\left\langle w_1\right|\left(I - |\Gamma_1\rangle\langle\Gamma_1| - |\Gamma_2\rangle\langle\Gamma_2|\right)\left|w_2\right\rangle\right| \\
&\leq 2\sqrt{1-(1-1/19)^2} \\
&\leq 13/20\,.
\end{aligned}$$

So orthogonalising $\{|w_j\rangle\} \to \{|w_j'\rangle\}$ gives – by Lemma 4.1.3 – a ground state overlap at least

$$1 - \frac{1 + 17/20}{1 - 17/20}\frac{1}{19} = 1 - 33/133 \geq 1 - 1/4\,.$$

This proves the required error bound. The number of spins i and cardinality p_1 is clearly unchanged by truncation, and the bond dimension is p_2 by definition. □

4.6 Error Reduction

The exact and approximate AGSPs are given respectively by

$$\begin{aligned}
A &:= \exp\left[-\frac{xH^2}{2\epsilon^2}\right] = \frac{\epsilon}{\sqrt{2\pi x}}\int_{-\infty}^{+\infty}\exp\left[-\frac{\epsilon^2 t^2}{2x} - iHt\right]\,\mathrm{d}t \\
K &:= \frac{2\epsilon}{\sqrt{2\pi x}}\sum_{j=0}^{T/\tau}\exp\left[-\frac{\epsilon^2\tau^2 j^2}{2x}\right]U_D(\tau j)\,.
\end{aligned}$$

If we take $x := 2\log(\zeta'^{-1}) = \mathcal{O}(\log \zeta^{-1})$ then the norm of A orthogonal to the ground space is bounded by $\zeta' := \zeta/70$. Following the analysis of Ref. [2], we have that K well-approximates A, specifically that

$$\|K - A\| \leq 3\zeta' .$$

As many of the approximation errors required to show this were stated without proof in Ref. [2] they have been explicitly calculated in Appendix C.

Take $|w_1\rangle$ and $|w_2\rangle$ to be the witnesses of $S_i^{(3)}$, such that they have ground state overlap at least $3/4$ and are orthonormal. First we look at what applying the exact AGSP will do to the energy:

Lemma 4.6.1. *For a $|w\rangle$ with ground state overlap at least $3/4$, taking $|v\rangle := A|w\rangle / \|A|w\rangle\|$, then $\langle v|H|v\rangle \leq 16\epsilon\zeta'^2$.*

Proof. Firstly decompose $|w\rangle$ into energy eigenstates

$$\sum_{j=0}^{d^n-1} \sqrt{p_j}\,|E_j\rangle$$

where $|E_j\rangle$ are all chosen to be non-degenerate, with increasing energy, such that $E_0 = 0$ and $E_j \geq \epsilon$ for $j \geq 1$. Normalisation gives that $\sum_j p_j = 1$. Applying the AGSP gives

$$\|A|w\rangle\|^2 \geq p_0 \|A|E_0\rangle\| = p_0 \geq 1/16$$

and so we can bound the energy of $|v\rangle$

$$\begin{aligned}\langle v|H|v\rangle &= \frac{\langle w|AHA|w\rangle}{\|A|w\rangle\|^2} \\ &\leq 16 \sum_j p_j E_j \exp\left(-xE_j^2/\epsilon^2\right) .\end{aligned}$$

Bounding all of the Gaussian terms by the largest, we have

$$\begin{aligned}&\leq 16 \left[\max_{E\geq\epsilon} E\exp(-xE^2/\epsilon^2)\right]\left[\sum_j p_j\right] \\ &\leq 16\epsilon\exp(-x) \\ &\leq 16\epsilon\zeta'^2 .\end{aligned}$$

□

The same arguments give that if the *approximate* AGSP is used – $|v\rangle := K|w\rangle / \|K|w\rangle\|$ – then this energy bound increases four-fold to $64\epsilon\zeta'^2$. Taking $|v_1\rangle := K|w_1\rangle / \|K|w_1\rangle\|$ and $|v_2\rangle := K|w_2\rangle / \|K|w_2\rangle\|$, the overlap between these two is bounded:

Lemma 4.6.2.

$$|\langle v_1|v_2\rangle| \leq 64\zeta'$$

Proof. Firstly, explicitly divide the approximate AGSP K into an AGSP term and an error term O, with $\|O\| = 1$

$$K = A + 3\zeta' O .$$

Thus the overlap is

$$\begin{aligned}|\langle v_1|v_2\rangle| &= \frac{\langle w_1|K^2|w_2\rangle}{\|K|w_1\rangle\|\,\|K|w_2\rangle\|} \\ &= 4\langle w_1|K^2|w_2\rangle \\ &= 4\langle w_1|\left[A^2 + 3\zeta' AO + 3\zeta' OA + 9\zeta'^2 O^2\right]|w_2\rangle .\end{aligned}$$

Using Cauchy-Schwarz on all but the A^2 term gives

$$\begin{aligned}&\leq 4\left\langle w_1\middle|A^2\middle|w_2\right\rangle + 12\zeta' + 36\zeta'^2\\&\leq 4\left\langle w_1\middle|A^2\middle|w_2\right\rangle + 48\zeta'\,.\end{aligned}$$

Using the orthogonality of $|w_1\rangle$ and $|w_2\rangle$, decomposing this into the ground and excitation components, its can be shown that $\left\langle w_1\middle|A^2\middle|w_2\right\rangle \leq 2\zeta'$ and so

$$|\langle v_1|v_2\rangle| \leq 56\zeta'\,.$$

□

Lemma 4.6.3. *Orthogonalising $\{v_i\} \to \{v_i'\}$ gives orthonormal witnesses of energy at most ζ.*

Proof. Applying Lemma 4.1.3 for overlap given above we get for $\zeta \leq 1$

$$\begin{aligned}\left\langle v_i'\middle|H\middle|v_i'\right\rangle &\leq 64\epsilon\zeta'^2\frac{1+56\zeta'}{1-56\zeta'}\\&\leq 70\zeta'\\&=:\zeta\,.\end{aligned}$$

□

Proof of Claim 4 The set $S_i^{(4)}$ is $(i,\, p(n)\,p_1(n),\, p(n)\,p_s(n),\, \Delta = c\epsilon^3)$-viable set.

Proof. The cardinality is increased by the number of A_j components used in the construction of K, i.e. the bond dimension of K as a matrix product operator, an operator formalism analogous to MPS. The scaling of D given in Section 3.4.4 gives that this cardinality is $p(n)$. Similarly, the relative increases in the bond dimensions of the witness states are also given by the bond dimension of K, namely $p(n)$. The error value is given above for $\zeta = c\epsilon^3$. □

For the $i = n$ case, by taking $\zeta = \eta/3$, we get the analogous result, whose proof is immediate.

Proof of Claim 5 The set $S_n^{(4)}$ is $(i,\, p_0(n)\,p_1(n),\, p_0(n)\,p_2(n),\, \Delta = \eta/3)$-viable set.

4.7 Final optimisation

Proof of Claim 6 The two resulting MPS vectors $|v_1\rangle$ and $|v_2\rangle$ are orthonormal, have bond dimension bounded by $p_0(n)$ given above, and ground state overlap at least $1-\eta$.

Proof. The two witnesses of the viable set $S_n^{(4)}$ serve as witnesses of this optimisation. As such both optimisations yield mixed states of energy at most $\eta/3$. As in Lemma 4.4.1 the leading eigenvector has an energy at most thrice the energy of the entire mixed state. As such, we conclude $\langle v_k|H|v_k\rangle \leq \eta$. As the two density matrices are orthogonal and positive, their constituent eigenvectors are all orthogonal, and thus the two resulting states are also orthogonal. □

Novelty is more important than correctness.
– Xiao-Gang Wen, *QFT of Many-Body Systems*

Chapter 5

Discussion and Conclusion

In this thesis we have generalised existing ground state algorithms to include degeneracy. The main original contribution is the orthogonalising size trimming procedure, which is necessary for a full set of witness states to be generated. The analysis of the difficulties in constructing degenerate viable sets – viz. the concept of left-distinguishability – is also original, and may prove important to further development of degenerate algorithms.

This work suggests two obvious open questions. The first is a rigorous proof of the full 1D degenerate area law, i.e. an extension from the state-of-the-art of Ref. [2] to the area law we used in Assumption 3.4.7. The second route for further research is the construction of a *frustrated* degenerate algorithm. Whilst the algorithm we have laid out is specific to unfrustrated systems, many of the steps can also be shown to function for frustrated systems. The main roadblock is the new size-trimming procedures, which – as described – rely heavily on a lack of frustration. This failure for unfrustrated systems is linked to the idea of left-distinguishability, and the fact that the local energy contributions of two ground states can differ (see Appendix E for more details).

Whilst our algorithm is constructed in the hope of laying the groundwork for a frustrated algorithm, even for unfrustrated systems it out-performs existing algorithms which rely far more heavily on this assumption. The algorithm of Ref. [4], for example, relies more heavily on the lack of frustration by taking the local Hamiltonian terms to be projectors. In doing so it is capable of efficiently approximating ground states of systems, but only if the half-chain degeneracy is polynomially bounded; our algorithm however requires no such bound. An example of a system for which this previous algorithm is inefficient, whilst ours is efficient, is given in Appendix D.

The link between an area law of entanglement and efficient ground state approximation algorithms raises the question as to whether there are more general links between structural and computational complexities. An example may be more general forms of simulation – such as time-evolution – for gapped 1D systems. Another possibility is similarly efficient simulations for other classes of systems known to possess area laws such as those with exponential decay of correlations [57, 58] or polynomial decay of specific heat [59].

Though our algorithm is efficient – running in polynomial time – it is far from practical, and little effort has been made to optimise the specific complexity. Reformulating the convex optimisations as semi-definite programs (SDP) for example would open much of the algorithm to the existing machinery for speeding up such SDPs, allowing for significant run-time improvements. Another possibility is that there may exist some algorithm that combines both the practical efficiency of heuristic methods, whilst maintaining the worst-case provable-efficiency of our algorithm.

Whilst the question of efficient ground state approximation may have been answered – in certain circumstances at least – the question of whether this can be done *locally* is still wide open. If one is concerned with the expectation of a localised observable for example, one may hope that simulating a region around that observable should be sufficient for its approximation. Whilst this may be possible with methods such as DMRG, the concept of a viable set so central to our algorithm is distinctly non-local. While we can easily extract the witness of a viable set defined on the entire spin chain, if it is only defined on some part of that chain however we cannot. Whether or not algorithms which possess the desired sense of locality exist, and how they relate to the structure-computational relationship, is still unknown.

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Appendix A

History of the 1D area law proofs

Hastings provided the first rigorous proof of the 1D area law in Ref. [13]. This proof was highly combinatorial, and relied on the eponymous Hastings' AGSP described above in Equation (B.3), as well as the Lieb-Robinson bound of Equation (2.1).

The main feature of entanglement leveraged however was the Coffman-Kundu-Wooters inequality [81], a result similar to a triangle inequality that bounds the entanglement between a region A and a combined region B_1B_2 by the entanglement between A and B_1/B_2 separately. Specifically it states

$$C^2_{AB_1} + C^2_{AB_2} \leq C^2_{A(B_1B_2)}$$

where C_{XY} is the *concurrence* [82], a measure of entanglement, between the regions X and Y. In the extreme case this gives that one region can only be maximally entangled to one other region, refered to as the *monogamy of entanglement* [83, 84]. The entanglement entropy bound across the cut $(j, j+1)$ found by Hastings was

$$S \leq c_0 \xi \log(6\xi) \log(d) 2^{6\xi \log(d)} = \tilde{\mathcal{O}}(64^{\xi \log d})$$

where ξ is the correlation length describe previously in Equation (2.2), and d the local dimension of the spins involved. In terms of the local dimension and gap alone the Hastings bound is

$$S \leq \exp\left(\mathcal{O}(\epsilon^{-1} \log d)\right)$$

The first improvement on this bound – in the unfrustrated case – came from Arad et.al. in Ref. [85]. In terms of the gap and local dimension and gap, the bound exponentially improved on that of Hastings

$$S \leq \mathcal{O}(1) \cdot (\epsilon^{-1} \log d)^3 \log^8(\epsilon^{-1} \log d) \leq \tilde{\mathcal{O}}(\epsilon^{-3} \log^3 d)$$

Their approached leveraged a more powerful AGSP construction, along with tighter limits on the entanglement generated by that AGSP, to gain a stronger entropy bound without the use of monogamy of entanglement. The specific construction involved splitting a Hamiltonian into local pieces and constructing a Chebyshev-based AGSP similar to that described in Section 2.5.1. A technical bound – known as the *detectability lemma* [49, 50] – was in turn used to bound the entanglement generated when projecting a product state arbitrary close to the ground state. Outside of 1D their result generalises to the bound on the entanglement entropy of a region A

$$S \leq \tilde{\mathcal{O}}\left(\epsilon^{-3} \log^3 d \, |\partial L|^2\right)$$

This is the first entropy bound that is purely dependent on the area (as opposed to the volume) in any dimension. Whilst this result gives area law scaling in one dimension, it reduces to a volume law in two or more dimensions. In two dimensions however this is tight, leaving this result right on the precipice of non-triviality.

Along with Kitaev, these authors were able to further improve [67] the gap dependence to give

$$S \leq \tilde{\mathcal{O}}(\epsilon^{-3/2} \log^3 d)$$

Much like the previous result this relied heavily on an AGSP construction. The construction used here however did not require for the Hamiltonian to be broken apart (i.e. it more closely conforms

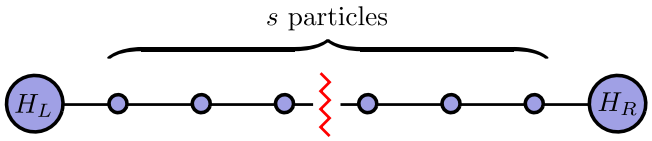

Figure A.1: The locally 1D system of Ref. [67]. Only $s \sim \log n$ particles were required to be arranged on a line, whilst the rest of the system is lumped together, here represented by H_L and H_R.

with the construction of Section 2.5.1), and polynomial interpolation techniques were used to avoid the necessity of the detectability lemma. As well as this, the proof was restructured in such a way that it only required that the system be *locally* 1D (see Figure A.1), utilising arguments similar to the decoupling found in 1D CSP algorithms of Section 2.4. An approximate form of this, termed the *truncation lemma*, was also shown to hold for the frustrated case, giving the same bound in this case as well.

All hitherto described proofs relied on the non-degeneracy of the Hamiltonian. The most recent positive result of Ref. [2] was found by strengthening previous lemmas surrounding the role of frustration to accommodate constant-degeneracy, giving the state-of-the-art bound

$$S \leq \tilde{\mathcal{O}}(\epsilon^{-1} \log^3 d)$$

Specifically it was shown that – for each cut – there exists a ground state which possesses this entanglement entropy across that cut. This result however did not prove there exists a ground state with this bound across *every* cut, nor that *every* ground state has that property; these results remain an open problem. As well as strengthening the gap dependence further, the techniques utilised were also able to be adapted for the Rényi entanglement entropy, yielding a far stronger form of area law. In terms of the gap alone[1], this bound is

$$R_\alpha \leq \tilde{\mathcal{O}}(\alpha^{-3}\epsilon^{-1}) \qquad \forall \alpha \in (0, 1]$$

which is precisely the ϵ-dependence we might intuitively expect from Figure 2.2.

[1] Whilst previously stated results were given in terms of the gap *and* local dimension for sake of completeness, the dependence on the latter in this case is rather complicated, and so has been omitted for clarity; the local dimension is considered a constant.

Appendix B

Alternative AGSP constructions

An approximate ground state projector (AGSP) [86] is an operator A which preserves ground states and shrinks excited states to a norm below δ, known as the AGSP's *shrinking factor*. By applying an AGSP and renormalising, the ground state overlap of a given state can be amplified [49]. The benefits over a true ground state projector is that they can be efficiently constructed, and can be constructed such that the amount of entanglement they incur is far less; in essence they are simpler operators. The specific construction is contextual, depending on the shrinking and entangling properties desired. We are going to discuss three such constructions here.

A simple AGSP utilised in the first polynomial-time ground state algorithm of Ref. [1] is given by a polynomial in the Hamiltonian.

$$A_p = \left(\frac{n - H}{n - E_0}\right)^m \tag{B.1}$$

which gives has a shriking factor of $\delta \approx \exp(-\Delta E \cdot m/n)$. The magnitude of the A_p AGSP, as it acts on energy eigenstates, is shown in Figure B.1(a).

Analytically, the problem with this AGSP is that the value of the exponent m required to give a desirable amount of shrinking will typically cause A_p to generate far too much entanglement. The algorithm of Ref. [1] got around this by not construction the whole operator, but sampling a polynomial number of terms from it, and utilising the matrix Chernoff bound [87]. Whilst this gives the desired bounds, it causes their algorithm to be stochastic in nature, something we wish to avoid.

Improving A_p can be framed in terms of a well-known problem in approximation theory. Ideally we wish for a polynomial whose value at $E = E_0$ is 1, and whose value for some range $E > E_1$ is very small; applying this polynomial would yield an AGSP similar to above. This relates strongly to the problem

$$\text{minimise} \max_{-1 \leq x \leq 1} |p(x)|$$

for a monic polynomial $p(x)$ of given order l, whose solution is given by the Chebyshev polynomial [88], most succinctly defined as

$$p_l(\cos\theta) = 2^{1-l} \cdot \cos(l\theta)$$

The extremal nature [89] of Chebyshev polynomials makes them ideal for an AGSP. The specific construction is

$$A_c := \frac{C_m(x)}{C_m(0)} \qquad C_m(x) := p_m\left(\frac{2x + m^2 + 1}{m^2 - 1}\right) \qquad x := \frac{H - E_0}{\Delta E} \tag{B.2}$$

The spectrum produced by the Chebyshev-base AGSP is shown in Figure B.1(b).

The AGSP used hereafter – the Hastings' AGSP[1] – is a tool which has been used to much success for gapped systems, in the analysis of both the exponential decay of correlations [14] and the 1D

[1] Known in Ref. [3] as the Hastings' MPO, where MPO is short for matrix product operator, an operator formalism analogous to the matrix product states of Section 2.7.2. For our purposes it only matters that it is an operator which can be efficiently represented.

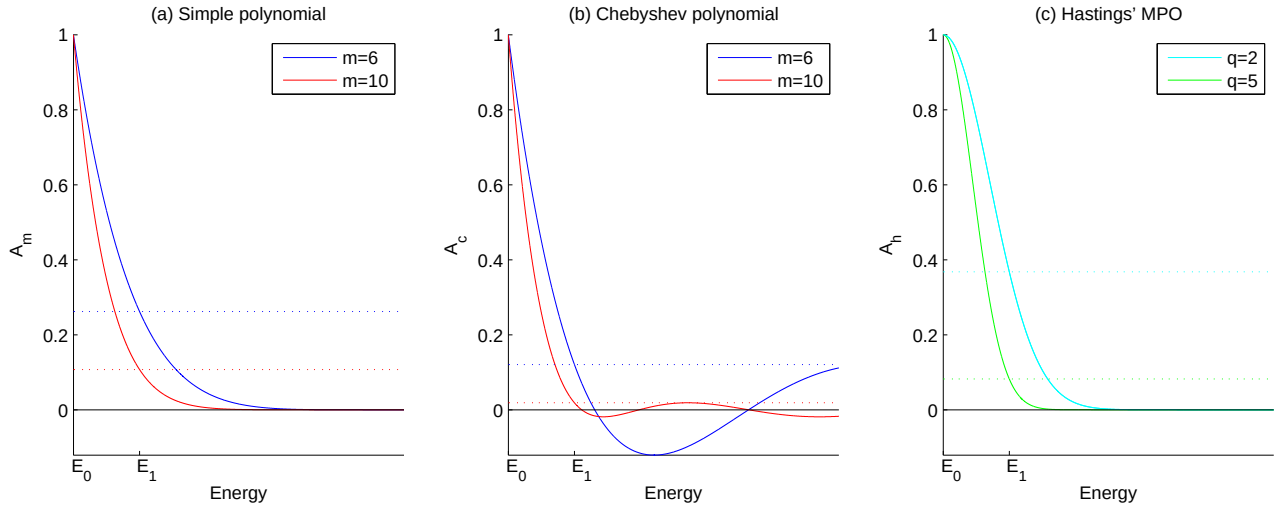

Figure B.1: The spectra for the AGSPs describe, as acting on energy eigenstates. The solid lines indicate the value for an energy eigenstate, the dotted lines the shrinking factors.

area law [13]. Its introduction to ground state algorithms was made in the state-of-the-art paper Ref. [3], and the analysis here follows that paper closely. The idea of the construction is to leverage the exponential decay of a Gaussian. Specifically let

$$A_h = \exp\left(-\frac{q(H-E_0)^2}{2\cdot\Delta E^2}\right) \tag{B.3}$$

with the analogous spectrum to the previous constructions is given in Figure B.1(c). The specific analysis of the various bounds on this AGSP, and the efficient approximation thereof, is given in Appendix C, with its application given in Section 3.4.4/4.6.

Appendix C

Hastings' AGSP Approximation

In this section we explicitly lay out the various errors associated with approximating Hastings' AGSP, as defined in Sections 3.4.4 and 4.6, and in Appendix B. The scaling of these errors was stated without proof in Ref. [3].

C.1 Definition

The AGSP is given by

$$A := \exp\left[-\frac{xH^2}{2\epsilon^2}\right] = \frac{\epsilon}{\sqrt{2\pi x}} \int_{-\infty}^{+\infty} \exp\left[-\frac{\epsilon^2 t^2}{2x} - iHt\right] \mathrm{d}t$$

and the approximate AGSP by

$$K := \frac{2\epsilon}{\sqrt{2\pi x}} \sum_{j=0}^{\lceil T/\tau \rceil} \exp\left[-\frac{\epsilon^2 \tau^2 j^2}{2x}\right] U_D(\tau j)$$

The magnitude on the excited subspace – the shrinking factor – is thus

$$\delta := e^{-x/2}$$

So if we take $\boxed{x := 2\log(\zeta'^{-1}) = \mathcal{O}(\log \zeta^{-1})}$ where $\zeta' := \zeta/70$ then this factor is ζ'.

C.2 Truncation error

The truncation error to the operator norm is due to the finite range of the integral, controlled by the parameter T. Its magnitude can be bounded

$$\begin{aligned}
\text{Truncation Error} &= 2\left|\frac{\epsilon}{\sqrt{2\pi x}} \int_{T}^{\infty} \exp\left[-\frac{\epsilon^2 t^2}{2x} - iHt\right] \mathrm{d}t\right| \\
&\leq \frac{2\epsilon}{\sqrt{2\pi x}} \int_{T}^{\infty} \exp\left[-\frac{\epsilon^2 t^2}{2x}\right] \mathrm{d}t \\
&= \frac{\epsilon}{\sqrt{2x}} \operatorname{erfc}\left(\frac{\epsilon T}{\sqrt{2x}}\right) \\
&\leq \frac{1}{T\sqrt{\pi}} \exp\left[-\frac{\epsilon^2 T^2}{2x}\right]
\end{aligned}$$

which can in turn be upper bounded by ζ' for the time-scale

$$\boxed{T := \frac{\sqrt{2x}}{\epsilon}\sqrt{\log \zeta'^{-1}} = \frac{2\log \zeta'^{-1}}{\epsilon} = \mathcal{O}(\epsilon^{-1} \log \zeta^{-1})}$$

C.3 Discretisation error

Next we consider the discretisation error associated with approximating this integral with a Riemann sum. The term being approximately integrated is a Gaussian centred on the origin and so it's modulus is even as a function of t, allowing us to consider only the $t > 0$ error and doubling it. On this range the modulus is not only even, but monotonically decreasing. As such the concepts of left and right Riemann sums correspond to upper and lower Riemann sums.

$$\text{Discretisation error} = 2\frac{\epsilon}{\sqrt{2\pi x}} \left\| \sum_{j=0}^{\lceil T/\tau \rceil} \tau \exp\left[-\frac{\epsilon^2\tau^2 j^2}{2x} - iH\tau j\right] - \int_0^T \exp\left[-\frac{\epsilon^2 t^2}{2x} - iHt\right] \mathrm{d}t \right\|$$

This error can be upper bounded in turn by the difference between upper and lower Riemann sums

$$\leq 2\frac{\epsilon\tau}{\sqrt{2\pi x}} \left\| \sum_{j=0}^{\lceil T/\tau \rceil} \exp\left[-\frac{\epsilon^2 t_j^2}{2x} - iH\tau j\right] - \sum_{j=1}^{\lceil T/\tau \rceil + 1} \exp\left[-\frac{\epsilon^2\tau^2 j^2}{2x} - iH\tau j\right] \right\|$$

As upper/lower are equivalent to left/right sums, this term becomes telescoping

$$\leq 2\frac{\epsilon\tau}{\sqrt{2\pi x}} \left\| 1 - \exp\left[-\frac{\epsilon^2 T^2}{2x} - iHT\right] \right\|$$

Taking the first-order Taylor series we can in turn bound this

$$\begin{aligned}
&\leq 2\frac{\epsilon\tau}{\sqrt{2\pi x}} \left\| 1 - \exp\left[-iHT\right] \right\| \\
&\leq 2\frac{\epsilon\tau}{\sqrt{2\pi x}} \left\| -iHT \right\| \\
&\leq 2\frac{\epsilon\tau T}{\sqrt{2\pi x}} \left\| H \right\| \\
&\leq 2\frac{\epsilon\tau T}{\sqrt{2\pi x}} n
\end{aligned}$$

Again this error can also be bounded by ζ' if we take the time-step

$$\boxed{\tau^{-1} := \frac{2\epsilon n T}{\zeta'\sqrt{2\pi x}} = 2n\zeta'^{-1}\sqrt{\frac{\log \zeta'^{-1}}{\pi}} = \mathcal{O}\left(n\zeta^{-1}\sqrt{\log \zeta^{-1}}\right)}$$

C.4 Trimming Error

To upper bound the total trimming error for the entire approximation by ζ', the trimming error for each propagator $\exp(-i\tau j)$ must be bounded by ζ', due to their additive nature. Using the construction of Ref. [77] this error can be achieved if the bond dimension of each propagator is

$$\begin{aligned}
D &= \exp\left[\mathcal{O}\left(\tau j\right) + \mathcal{O}\left(\log n/\zeta'\right)\right] \\
&\leq \exp\left[\mathcal{O}\left(T\right) + \mathcal{O}\left(\log n/\zeta\right)\right] \\
&= e^{\mathcal{O}(T)}\mathsf{poly}(n/\zeta) \\
&= (1/\zeta)^{\mathcal{O}(1/\epsilon)}\,\mathsf{poly}(n/\zeta)
\end{aligned}$$

which in turn gives a total bond dimension for the AGSP on the order of

$$\begin{aligned}
B &\leq 2T\tau^{-1}D \\
&= \frac{8n\zeta^{-1}\log^{3/2}(3/\zeta)}{\sqrt{\pi}\epsilon} \cdot (1/\zeta)^{\mathcal{O}(1/\epsilon)} \cdot \mathsf{poly}(n/\zeta) \\
&= (1/\zeta)^{\mathcal{O}(1/\epsilon)} \cdot \mathsf{poly}(n/\zeta)
\end{aligned}$$

Appendix D

Constant-fold degenerate system with exponential half-chain degeneracy

The example we use is based on a modified Ising model [79]. To do this we take the Ising model and add extra local degrees of freedom, which we couple to one of the ground states. The two ground states of the ferromagnetic Ising model, $|000\ldots\rangle$ and $|111\ldots\rangle$, are locally distinguishable, so we can then push all of these extra local degrees of freedom out of the ground space with a local perturbation. This will allow for a single perturbed local term to exponentially change the degeneracy. The qubit Ising model on a line is defined via $H = -\sum_{j=1}^{n-1} Z_j Z_{j+1}$, where Z is the Pauli-Z operator. Consider taking each single-qubit operator Z, and extending it to a qutrit (3-level system) operator ζ, which interacts identically with the $|1\rangle$ and $|2\rangle$ computational basis states.

$$Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \rightarrow \quad \zeta := \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Replacing the Hamiltonian terms with $\zeta_j \zeta_{j+1}$ – now acting on a qutrit chain of the same geometry – the modified ground states now become

$$\begin{aligned} |000\ldots\rangle \quad &\rightarrow \quad |000\ldots\rangle \\ |111\ldots\rangle \quad &\rightarrow \quad \begin{cases} |111\ldots\rangle \\ |211\ldots\rangle \\ |121\ldots\rangle \\ \quad\vdots \\ |222\ldots\rangle \end{cases} \end{aligned}$$

As a result the degeneracy of this modified Ising model is $2^n + 1$. By adding a one-body term $-\zeta_1$ on the beginning of the chain, we drop this exponential degeneracy down to a constant on the whole system, with $|000\ldots\rangle$ being the unique ground state. However, if we instead add $-\zeta_i$ on the ith qutrit instead, the *half-chain* degeneracy of the first i spins $g_{[1,i]}$ is generally exponential,

$$g_{[1,i]} = \begin{cases} 2^i + 1 & \text{for } i < n \\ 1 & \text{for } i = n \end{cases}.$$

This model is related to work done by Hastings in Ref. [80], in which the relationship between entanglement entropy and the correlation length is studied. As shown in Hastings area law of Ref. [13] of the same year, the entropy can grow exponentially in the correlation length, which is the case for this system. This exponential growth can be related, at least in this case, to the half-chain degeneracy.

Appendix E

Frustration bound

Lemma E.1. *Suppose H is a 1D local Hamiltonian comprised of two-body terms H_i with $H_i \geq 0$ and $\|H_i\| \leq 1$, with degenerate ground states $|\Gamma_1\rangle$ and $|\Gamma_2\rangle$. For any given cut, the expectation value of the Hamiltonian terms to the left of that cut H_L for the two ground states differs by at most one unit of energy.*

Proof. Fix an i at the cut, and split the Hamiltonian in terms entirely to the left of the cut, across the cut, and to the right of the cut.

$$H_L := \sum_{j=0}^{i-1} H_j \qquad H_M := H_i \qquad H_R := \sum_{j=i+1}^{n-1} H_j$$

Next Schmidt decompose the two ground states across the given cut

$$|\Gamma_1\rangle = \sum_k \lambda_{1,k} |a_{1,k}\rangle \otimes |b_{1,k}\rangle \qquad |\Gamma_2\rangle = \sum_k \lambda_{2,k} |a_{2,k}\rangle \otimes |b_{2,k}\rangle$$

Let $E := \langle\Gamma_1|H|\Gamma_1\rangle = \langle\Gamma_2|H|\Gamma_2\rangle$. Letting $E_L := \langle\Gamma_1|H_L|\Gamma_1\rangle$ and $\Delta = \langle\Gamma_2|H_L|\Gamma_2\rangle - E_L$. Without loss of generality we can take Γ_2 to have a left energy no smaller than Γ_1 and thus restrict $\Delta \geq 0$. By contradiction assume further that $\Delta > 1$.

As E_L is simply a weighted average of the energies of the left Schmidt vectors $a_{1,k}$

$$\begin{aligned} E_L &= \langle\Gamma_1|H_L|\Gamma_1\rangle \\ &= \sum_{k,k'} \lambda^*_{1,k}\lambda_{1,k'} \langle a_{1,k}|H_L|a_{1,k'}\rangle \langle b_{1,k}|I|b_{1,k'}\rangle \\ &= \sum_k |\lambda_{1,k}|^2 \langle a_{1,k}|H_L|a_{1,k}\rangle \end{aligned}$$

then there must exist a left Schmidt vector $|A\rangle$ of $|\Gamma_1\rangle$ such that $\langle A|H_L|A\rangle \leq E_L$. Similarly we can see that

$$\begin{aligned} \langle\Gamma_2|H_R|\Gamma_2\rangle &= E - \langle\Gamma_2|H_M|\Gamma_2\rangle - \langle\Gamma_2|H_R|\Gamma_2\rangle \\ &= E - E_L - \Delta - \langle\Gamma_2|H_M|\Gamma_2\rangle \\ &\leq E - E_L - \Delta \end{aligned}$$

which also implies that there exists a right Schmidt vector $|B\rangle$ of $|\Gamma_2\rangle$ with $\langle B|H_R|B\rangle \leq E - E_L - \Delta$. Consider the product state made from these two vectors:

$$|v\rangle := |A\rangle \otimes |B\rangle$$

The energy of this state is

$$\begin{aligned} \langle v|H|v\rangle &= \langle v|H_L|v\rangle + \langle v|H_M|v\rangle + \langle v|H_R|v\rangle \\ &= \langle A|H_L|A\rangle + \langle B|H_R|B\rangle + \langle v|H_M|v\rangle \\ &\leq E_L + E - E_L - \Delta + 1 \\ &= E - \Delta + 1 \\ &< E \end{aligned}$$

And thus v is a state with an energy strictly lower than the ground energy. Thus by contradiction we can see that $\Delta > 1$ was not possible and thus that the expectation of the left Hamiltonians can not differ by more than $\|H_i\|$; one unit of energy. □

Corollary E.2. *For the same Hamiltonian and ground states in the previous Lemma, taking H_V to be the Hamiltonian terms entirely supported in a region V, then the expectation value $\langle H_V \rangle$ of the ground states can differ, at most, by ∂V (Not including boundary elements at the edge of the chain).*

Proof. The proof is analogous to the case above. The states once again can be repeatedly Schmidt decomposed along each boundary and then a product state can be constructed whose energy is less than the piecewise minimum, plus excitations corresponding to the boundary terms. As such if the expectations of H_V differ by more than ∂V then these excitations cannot account for the product states energy, and thus to avoid contribution the desired bound must hold. □

Lemma E.3. *The above lemma is tight.*

Proof. Consider the Ising model on 4 qubits with frustrating perturbations on each end:

$$\begin{aligned} H_1 &= \frac{3}{2}I - \frac{1}{2}Z_1 - Z_1Z_2 \\ H_2 &= I - Z_2Z_3 \\ H_3 &= \frac{3}{2}I + \frac{1}{2}Z_4 - Z_3Z_4 \end{aligned}$$

with the ground states $|\Gamma_1\rangle = |0000\rangle$ and $|\Gamma_2\rangle = |1111\rangle$. The energies are thus

$$\begin{aligned} \langle\Gamma_1|H_1|\Gamma_1\rangle &= 0 & \langle\Gamma_2|H_1|\Gamma_2\rangle &= 1 \\ \langle\Gamma_1|H_2|\Gamma_1\rangle &= 0 & \langle\Gamma_2|H_2|\Gamma_2\rangle &= 0 \\ \langle\Gamma_1|H_3|\Gamma_1\rangle &= 1 & \langle\Gamma_2|H_3|\Gamma_2\rangle &= 0 \end{aligned}$$

and so the left energies differ by the maximally allowed value of 1. A similar example could be constructed for any region V by placing on-site $+Z$ terms in each connected component of V and on-site $-Z$ terms in each connected component of the complement. □