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**Classical simulation of quantum many-body systems**

by

Yichen Huang

A dissertation submitted in partial satisfaction of the

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University of California, Berkeley

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Professor Joel E. Moore, Chair

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# Classical simulation of quantum many-body systems

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Yichen Huang

## Abstract

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Doctor of Philosophy in Physics

University of California, Berkeley

Professor Joel E. Moore, Chair

Classical simulation of quantum many-body systems is in general a challenging problem for the simple reason that the dimension of the Hilbert space grows exponentially with the system size. In particular, merely encoding a generic quantum many-body state requires an exponential number of bits. However, condensed matter physicists are mostly interested in local Hamiltonians and especially their ground states, which are highly non-generic. Thus, we might hope that at least some physical systems allow efficient classical simulation.

Starting with one-dimensional (1D) quantum systems (i.e., the simplest nontrivial case), the first basic question is: Which classes of states have efficient classical representations? It turns out that this question is quantitatively related to the amount of entanglement in the state, for states with “little entanglement” are well approximated by matrix product states (a data structure that can be manipulated efficiently on a classical computer). At a technical level, the mathematical notion for “little entanglement” is area law, which has been proved for unique ground states in 1D gapped systems. We establish an area law for constant-fold degenerate ground states in 1D gapped systems and thus explain the effectiveness of matrix-product-state methods in (e.g.) symmetry breaking phases. This result might not be intuitively trivial as degenerate ground states in gapped systems can be long-range correlated.

Suppose an efficient classical representation exists. How can one find it efficiently? The density matrix renormalization group is the leading numerical method for computing ground states in 1D quantum systems. However, it is a heuristic algorithm and the possibility that it may fail in some cases cannot be completely ruled out. Recently, a provably efficient variant of the density matrix renormalization group has been developed for frustration-free 1D gapped systems. We generalize this algorithm to all (i.e., possibly frustrated) 1D gapped systems. Note that the ground-state energy of 1D gapless Hamiltonians is computationally intractable even in the presence of translational invariance.

It is tempting to extend methods and tools in 1D to two and higher dimensions (2+D), e.g., matrix product states are generalized to tensor network states. Since an area law for entanglement (if formulated properly) implies efficient matrix product state representations in 1D, an interesting question is whether a similar implication holds in 2+D. Roughly speaking,

we show that an area law for entanglement (in any reasonable formulation) does not always imply efficient tensor network representations of the ground states of 2+D local Hamiltonians even in the presence of translational invariance. It should be emphasized that this result does not contradict with the common sense that in practice quantum states with more entanglement usually require more space to be stored classically; rather, it demonstrates that the relationship between entanglement and efficient classical representations is still far from being well understood.

Excited eigenstates participate in the dynamics of quantum systems and are particularly relevant to the phenomenon of many-body localization (absence of transport at finite temperature in strongly correlated systems). We study the entanglement of excited eigenstates in random spin chains and expect that its singularities coincide with dynamical quantum phase transitions. This expectation is confirmed in the disordered quantum Ising chain using both analytical and numerical methods.

Finally, we study the problem of generating ground states (possibly with topological order) in 1D gapped systems using quantum circuits. This is an interesting problem both in theory and in practice. It not only characterizes the essential difference between the entanglement patterns that give rise to trivial and nontrivial topological order, but also quantifies the difficulty of preparing quantum states with a quantum computer (in experiments).

To my parents,

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Perhaps you have already noticed that I am keeping names as implicit as possible. This is for a mild protection of privacy.

# Chapter 1

## Introduction

### 1.1 Motivation and background

The main object of study in condensed matter physics is quantum many-body systems, i.e., a system of a very large (or even an infinite) number of particles (or spins) governed by the laws of quantum mechanics. In addition, particles are usually arranged in a regular lattice, and they typically have short-range interactions. Such a situation gives rise to the notion of a local Hamiltonian. A local Hamiltonian is a Hermitian operator of the form  $H = \sum_i H_i$ , where each term  $H_i$  acts non-trivially only on a small constant number of particles. Although  $H$  is a matrix of dimension exponential in the system size, its description in terms of each individual term is efficient because there are at most a polynomial number of terms.

The goal is to study the physics of local Hamiltonians. Besides the time evolution (governed by the Schrodinger equation) and thermal properties (described by the canonical ensemble), the ground state (i.e., the eigenvector of  $H$  with the smallest eigenvalue) is of the most fundamental interest, as it is the state of matter when the system is cooled to zero (or very low compared to the energy gap) temperature. For instance, one might wish to estimate the ground-state energy (i.e., the smallest eigenvalue of  $H$ ) or to compute two-point correlation functions for the ground state. Indeed, the ground states of local Hamiltonians can exhibit a variety of exotic phases of matter including the quantum Hall effect and the high-temperature superconductors. Thus, understanding the physics of local Hamiltonians is an essential step towards designing new, advanced materials with desirable properties.

This dissertation studies local Hamiltonians (mostly) with a classical computer. Given a local Hamiltonian  $H$ , we ask questions such as:

1. Can objects of interest, especially the ground state of  $H$ , be represented by a space-efficient data structure? Can physical properties be efficiently extracted from such a space-efficient data structure?
2. Is there an efficient algorithm for finding such a space-efficient (classical) representation?
3. Can we quantify the hardness of determining certain properties of local Hamiltonians by establishing connections to computational complexity theory?

As a side remark, an efficient algorithm to a physicist typically means a heuristic algorithm that is fast in practice, while an efficient algorithm to a computer scientist usually means a rigorous algorithm that runs in polynomial time in worst cases.

The main technical challenge comes from the simple observation that the dimension of the Hilbert space grows exponentially with the system size. Specifically, we would like to compute the physical properties of local Hamiltonians, which are square matrices of exponential dimension, whereas an efficient algorithm must run in polynomial time. Despite this challenge, a lot of progress has been made in the past decade, especially for one-dimensional (1D) quantum systems.

Before closing this section, we would like to point out that quantum simulation (i.e., simulating quantum systems efficiently with quantum devices [43]) is another very exciting field of research [35]. Note that quantum simulation does not require a universal quantum computer; rather, a device tailored to the doped Hubbard model would suffice to demystify high-temperature superconductivity. Unfortunately, quantum simulation will not be covered in this dissertation.

## 1.2 Organization and overview

This dissertation assumes almost no prior knowledge in condensed matter theory (e.g., it is not necessary to know the phase diagram of the 1D transverse field Ising model), but requires a solid background in quantum mechanics. Thus, it is accessible to any graduate student in physics.

Chapter 2 is a gentle review of preliminary knowledge in the field. It begins with an introduction to basic and important techniques for simulating quantum many-body systems, such as matrix product states (MPS), density matrix renormalization group (DMRG; here, the word “group” does not refer to a group in mathematics), and tensor network states. We then discuss area laws, which are a set of theorems and conjectures about the entanglement in various interesting classes of quantum states. We close this chapter with a mini-survey of the computational complexity of the local Hamiltonian problem. The materials in this chapter (and Section 1.1) are extracted from the review article available on arXiv [49] (and has been accepted for publication as a monograph in *Foundations and Trends in Theoretical Computer Science*).

The bulk (i.e., remainder) of this dissertation is a collection of my papers (with collaborators) in 2014. Before 2014, I had worked on quantum entanglement [72, 75, 73], quantum information [76, 71], quantum mechanics [74, 78], and other topics in condensed matter theory [80, 77]. These papers are not included in this dissertation as they are outside the scope of my current research.

We now give a chapter-by-chapter overview of the bulk of this dissertation. Each chapter stands on its own and can be read independently from others.

Since the technical challenge is forbidding, we must resort to the most humble scientific method: starting with the simplest nontrivial case. In particular, we mainly study 1D quan-

tum systems, in which the DMRG algorithm is remarkably successful in practice. However, DMRG is a heuristic algorithm: There is no guarantee that it never gets stuck in local minima, nor that it always converges rapidly. Since DMRG is a variational algorithm over MPS, we ask: First, which classes of states can be efficiently represented as (or approximated by) MPS? Second, if an efficient MPS representation exists, can one find it efficiently?

The first question is quantitatively related to the amount of entanglement in the state: Indeed, states with “little entanglement” are well approximated by MPS. It has been proved that the entanglement (across any cut) of unique ground states in 1D gapped systems is upper bounded by a constant independent of the system size [59, 10]. This is known as an area law. Chapter 3 extends the area law to 1D gapped systems with constant-fold ground-state degeneracy and thus explains the effectiveness of DMRG in (e.g.) symmetry breaking phases. In particular, we show that any state in the ground-state space satisfies an area law. This chapter also includes some technical improvements to the previous results [59, 10] for unique ground states. This chapter is available on arXiv [70].

On the second question, very important progress for frustration-free systems was made in [95]. Chapter 4 extends this result to a (provably) deterministic polynomial-time algorithm for computing the ground-state wave function of any (i.e., possibly frustrated and non-translationally invariant) 1D gapped Hamiltonian. In the case that the ground states are constant-fold degenerate, the algorithm returns a basis of the ground-state space. As a consequence, 1D adiabatic quantum computation allows efficient classical simulation if the final Hamiltonian is gapped, improving the result of Hastings [61] which requires a constant energy gap along the path of Hamiltonians. This chapter is available on arXiv [69].

Quantum many-body systems in two and higher dimensions (2+D) can host a variety of exotic phases of matter including the quantum Hall effect and the high-temperature superconductors. Thus, they are much more exciting to physicists. They are also much more challenging from a technical perspective, and indeed there are a lot of important open problems. For example, a famous conjecture in the community is that the ground states of gapped local Hamiltonians in any spatial dimension satisfy an area law for entanglement, but a proof of (or a counterexample to) this conjecture appears very difficult.

It is well known that an area law for entanglement (if formulated properly) implies efficient MPS representations in 1D, and it was commonly believed that a similar implication holds in 2+D: An area law implies efficient tensor network state representations. In contrast to the belief, it was recently proved that there exist (translationally invariant) quantum many-body states satisfying area laws but do not have efficient tensor network representations [48]. Under a very mild and widely accepted assumption in quantum complexity theory, Chapter 5 establishes a similar result with an additional important physical property: there exist (translationally invariant) local Hamiltonians whose ground states satisfy area laws but do not have efficient tensor network representations. This chapter is available on arXiv [68].

Excited eigenstates are physical states participating in the dynamics of quantum systems. They become particularly relevant in the context of many-body localization as localization is a (dynamic) property associated with all eigenstates (not just the ground state) of disordered systems. Chapter 6 studies the singularities of the entanglement of excited eigenstates in

random spin chains using both analytical (renormalization group) techniques and numerical simulations. In the random quantum Ising chain, we find that the entanglement of (almost) all eigenstates becomes singular at the quantum critical point, which strongly suggests that the zero-temperature quantum phase transition is also a dynamical phase transition. This chapter was published as a Rapid Communication in *Physical Review B* [81].

Finally, we study the problem of generating the ground states of 1D gapped Hamiltonians using quantum circuits. Although this problem is not directly related to classical simulation (of quantum many-body systems), it is still marginally relevant to the scope of this dissertation as quantum circuits provide a powerful tool for quantitatively characterizing the entanglement patterns of topologically ordered states. Also, the quantum circuit complexity of generating quantum states (from product states) is a fundamental problem describing the difficulty of preparing quantum states with a quantum computer (in experiments).

It was argued that topological order is essentially a pattern of long-range entanglement. Although such an entanglement point of view has led to important advances in understanding topological order and has been widely accepted by the community, a quantitative characterization of long-range entanglement is still not totally clear. Quantum circuits provide a new perspective on classifying entanglement patterns (or topological order). In particular, it was defined in [31] that a quantum state is short-range entangled if it can be generated from a product state via a local quantum circuit of constant depth, suggesting that short-range entanglement is just local rearrangement of quantum correlations.

Intuitively, topologically ordered (i.e., long-range entangled) states have global quantum correlations. In 1D, Chapter 7 makes this intuition precise by showing that to generate states with nontrivial topological order (from product states) local quantum circuits of linear (in the system size) depth are necessary and (up to reasonably small errors) sufficient. This result holds for both fermionic and (bosonic) spin systems and for all symmetry protected topological phases (where we use symmetric circuits). This chapter is available on arXiv [79] (and has been accepted for publication as a long article in *Physical Review B*).

### 1.3 List of acronyms

1D	one dimension
2D	two dimensions
3D	three dimensions
2+D	two and higher dimensions
MPS	matrix product state
PEPS	projected entangled pair state
MERA	multi-scale entanglement renormalization ansatz
DMRG	density matrix renormalization group
NP	nondeterministic polynomial
QMA	quantum Merlin Arthur
SPT	symmetry protected topological (phase)

# Chapter 2

## Preliminaries

In this chapter, we give a brief introduction to basic concepts and techniques that are relevant to the bulk of this dissertation.

### 2.1 Matrix product state

As the simplest class of tensor network states, MPS is a very useful ansatz of trial wave functions. It plays a fundamental role not only in the classical simulation of 1D quantum systems [155, 156], but also in the classification of (symmetry protected) topological phases [29, 136]. Consider a chain of  $n$  spins, each of which has local dimension  $d = \Theta(1)$ . We associate each site  $i$  with  $d$  matrices  $A_i^{[j]}$  for  $j = 1, 2, \dots, d$ . In the bulk  $2 \leq i \leq n - 1$ , each  $A_i^{[j]}$  is of dimension  $D \times D$ ; at the boundaries, each  $A_1^{[j]}$  is of dimension  $1 \times D$  and each  $A_n^{[j]}$  is of dimension  $D \times 1$ . An MPS takes the form

$$|\psi\rangle = \sum_{j_1, j_2, \dots, j_n=1}^d A_1^{[j_1]} A_2^{[j_2]} \dots A_n^{[j_n]} |j_1 j_2 \dots j_n\rangle. \quad (2.1)$$

Since  $A_1^{[j_1]}$  and  $A_n^{[j_n]}$  are row and column vectors, respectively, the expression  $A_1^{[j_1]} A_2^{[j_2]} \dots A_n^{[j_n]}$  is a (complex) number, which is the amplitude of  $|j_1 j_2 \dots j_n\rangle$ . As such, the amplitudes are encoded as products of matrices, justifying the name “matrix product state”. The index  $j_i$  is referred to as a physical index, as it corresponds to the physical degrees of freedom (at the site  $i$ ).

The value  $D$  is called the bond dimension. Using singular value decompositions, it is easy to see that any state  $|\psi\rangle$  can be expressed exactly as an MPS if the bond dimension  $D$  is large enough. Indeed, it suffices that  $D$  is the maximum Schmidt rank of  $|\psi\rangle$  across any cut. In general, such a value of  $D$  is not computationally feasible as it grows exponentially with  $n$ . However, the strength of MPS is that any state with “little entanglement” (across any cut) is well approximated by an MPS with small  $D$ . This feature of MPS turns out to be very essential, as condensed matter physicists are mainly interested in the ground states of local

Hamiltonians, which are highly non-generic. For example, in 1D gapped systems we have an area law [59, 10, 70], implying that the entanglement across any cut is upper bounded by a constant independent of  $n$ . In 1D conformally invariant critical (gapless) systems, the area law is slightly violated with a logarithmic factor  $\sim \log n$  [66, 28, 27], suggesting that MPS is still a fairly efficient parametrization.

Another key property of MPS is that it supports efficient computation of physical observables, such as energy, (expectation values of) order parameters, correlation functions, and even entanglement entropy [133]. This is in contrast to more complicated tensor network states such as PEPS, which are in general  $\#P$ -hard to contract [138].

## 2.2 Density matrix renormalization group

The DMRG algorithm is nowadays considered the most powerful numerical method for 1D quantum systems. In many applications of DMRG, we are able to obtain the physics (e.g., the ground-state energy, ground-state correlation functions) of a 1D quantum lattice model with extraordinary precision and moderate computational resources. Historically, White’s invention of DMRG [161, 162] two decades ago was stimulated by the failure of Wilson’s numerical renormalization group [163] for homogeneous systems. Subsequently, a milestone was achieved when it was realized [115, 131, 150, 109] that DMRG is a variational algorithm over MPS.

The purpose of this section is to sketch at a high level how DMRG works from the MPS point of view. For further details, we refer the reader to the following review papers on the topic. Ref. [133] is a very detailed account of coding with MPS. The earlier paper [132] discusses DMRG mostly in its original formulation. Refs. [149, 34] focus on the role MPS plays in DMRG, as well as other variational classes of states, such as tree tensor network states [140], PEPS [147] and MERA [153].

The idea behind DMRG from the MPS perspective is as follows. Given an input Hamiltonian  $H$ , we minimize the energy  $\langle \psi | H | \psi \rangle$  with respect to all MPS  $|\psi\rangle$  of some bond dimension  $D$ , i.e., with respect to  $O(ndD^2)$  parameters ( $n$  is the system size). In general,  $D$  has to grow with  $n$  (especially in critical or gapless systems). Unfortunately, minimizing the energy for  $D = \text{poly}(n)$  can be NP-hard even for frustration-free Hamiltonians [134]. To cope with this, DMRG is a heuristic algorithm for finding local minima. There is no guarantee that the local minima we find are global minima, nor that the algorithm converges rapidly. However, perhaps surprisingly, in practice DMRG works fairly well even in critical systems.

At a high level, the DMRG algorithm proceeds as follows. We start with an MPS denoted by a collection of matrices  $\{A_i^{[j]}\}_{i=1,2,\dots,n}^{j=1,2,\dots,d}$  and then perform a sequence of local optimizations. A local optimization at site  $i_0$  means minimizing the energy  $\langle \psi | H | \psi \rangle$  with respect to the matrices  $\{A_i^{[j]}\}_{i=i_0}^{j=1,2,\dots,d}$  associated with the site, while keeping all other matrices  $\{A_i^{[j]}\}_{i \neq i_0}^{j=1,2,\dots,d}$  fixed. These local optimizations are performed in a number of “sweeps” until the solution  $\{A_i^{[j]}\}_{i=1,2,\dots,n}^{j=1,2,\dots,d}$  converges. Here, a sweep consists of local optimizations applied in sequence

starting at site 1 up to site  $n$ , and then backwards back to site 1, i.e., in a sweep we apply the local optimizations in the following order of sites:  $1, 2, \dots, n-1, n, n-1, \dots, 2, 1$ .

## 2.3 Tensor network states

Since tensor network states are usually constructed as trial wave functions, we begin this section with a brief discussion of the variational principle. As a heuristic method, the main idea of the variational principle is as follows. Suppose we would like but it is difficult to optimize a function  $f$  over a set  $S$ . Our strategy is to do the optimization over some subset  $S' \subseteq S$ . We wish that (i) the optimization over  $S'$  is (in some sense) close to the optimization over  $S$ ; (ii) performing the optimization over  $S'$  is technically easier. In the context of this section, we would like to compute the ground-state wave function  $|\psi\rangle$  by minimizing the energy  $\langle\psi|H|\psi\rangle$ . Apparently, a generic state  $|\psi\rangle$  requires an exponential number of bits to describe. This is an obstacle for designing a heuristic method to minimize the energy. Using the variational principle, we can instead minimize over a simpler set  $S'$  of certain physically relevant quantum states to approximate the ground-state energy. The key is of course to decide which set  $S'$  of states we should choose.

For example, one may choose  $S'$  as the set of product states. This simple ansatz, known as mean-field theory, turns out to be quite effective in many scenarios. Note that working with product states is in general still a hard problem. It is easy to see that minimizing the energy over product states is NP-hard. Indeed, a quantum Hamiltonian becomes a classical Hamiltonian if each term is diagonal in the computational basis, and finding the ground state (which must be a product state) of a classical Ising spin glass is NP-hard [13].

One may choose  $S'$  as the set of tensor network states [149]. Unlike product states, which have absolutely no entanglement or correlations, tensor network states can represent a variety of exotic quantum phases of matter, such as those with (even chiral [38, 159]) topological order [151, 2]. However, contracting tensor networks is in general #P-hard [138]. One strategy to circumvent this is to choose a subset  $S''$  of tensor network states which support efficient computation of physical observables. The most successful application of the variational principle based on tensor network states is the DMRG algorithm as a variational algorithm over MPS.

We now give an informal definition of tensor network states. Suppose you were a software engineer at the moment. A  $k$ -dimensional tensor (or  $k$ -tensor for short)  $M(i_1, i_2, \dots, i_k)$  is a  $k$ -dimensional array of complex numbers. For instance, in the language of linear algebra, a 1-tensor is a vector, and a 2-tensor is a matrix. Note that we often denote indices as super- or sub-scripts, e.g., a 3-tensor  $M(i_1, i_2, i_3)$  can be denoted by  $M_{i_3}^{i_1, i_2}$ . The bond dimension of a tensor is the maximum number of different values any index can take.

The contraction of two tensors is defined as follows. Suppose we are given two 3-tensors  $M(i_1, i_2, i_3)$  and  $N(j_1, j_2, j_3)$ . Their contraction on the middle indices yields a 4-tensor  $P$ :

$$P(i_1, i_3, j_1, j_3) = \sum_k M(i_1, k, i_3)N(j_1, k, j_3). \quad (2.2)$$



Any quantum state  $|\psi\rangle$  of  $n$  spins (each of which has local dimension  $d$ ) can be identified with an  $n$ -tensor of bond dimension  $d$ . Indeed, by expanding  $|\psi\rangle = \sum_{i_1, i_2, \dots, i_n=1}^d \alpha_{i_1, i_2, \dots, i_n} |i_1 i_2 \dots i_n\rangle$  in the computational basis, we define an  $n$ -tensor  $M$  such that  $M(i_1, i_2, \dots, i_n) = \alpha_{i_1, i_2, \dots, i_n}$ . The state  $|\psi\rangle$  is called a tensor network state if the  $n$ -tensor  $M$  can be expressed as the contraction of a network of  $c$ -tensors, where  $c$  is a small absolute constant. The bond dimension of the tensor network is defined as the maximum bond dimension of each  $c$ -tensor.

Tensor network states include as special cases MPS [118], MERA [153], and PEPS [147]. Indeed, an MPS can be expressed as the contraction of a line of 3-tensors, and on a 2D square lattice a PEPS can be expressed as the contraction of 5-tensors. Note that MPS and MERA [152] can be contracted efficiently, but contracting PEPS is #P-complete [138].

The bond dimension  $D$  determines the space complexity of tensor network states. Apparently, the larger  $D$  is, the more quantum states we can represent, at the price of more storage space. In practice, we should keep the bond dimension as small as possible. Since representing a generic quantum state requires exponential bond dimension, a key question is: *Which quantum many-body systems have ground states that are well approximated by tensor network states of small bond dimension?*

We now briefly review recent progress on this question and related algorithmic advances. In 1D gapped systems, Hastings [59] first proved that MPS of polynomial bond dimension approximate the ground state well. Indeed, MPS of polynomial bond dimension approximate the ground state well as long as certain Renyi entanglement entropy diverges at most logarithmically [146] (see also [139]). These results give an intuitive explanation of the effectiveness of DMRG as a variational algorithm over MPS, although DMRG remains heuristic. To develop a rigorous variant of DMRG that is provably efficient in all 1D gapped systems, it was first realized that the optimal MPS of constant bond dimension can be found efficiently via dynamic programming [5, 135]. This algorithm does not require the Hamiltonian to be gapped, but its running time grows exponentially with the bond dimension. For 1D gapped systems with energy gap  $\epsilon$ , Arad, Kitaev, Landau and Vazirani [10] improved Hastings' result by showing that MPS of sub-polynomial bond dimension  $D = \exp(\tilde{O}(\epsilon^{-1/4} \log^{3/4} n))$  approximate the ground state well, where  $\tilde{O}(x) := O(x \text{ poly log } x)$  hides a polylogarithmic factor. In the case that the ground states are constant-fold degenerate, any state in the ground-state space allows MPS approximations with the same scaling of the bond dimension [70]. Combined with the algorithms of [5, 135], this immediately implies a sub-exponential time algorithm for 1D gapped systems. Finally, a polynomial-time algorithm for computing MPS approximations to ground states in 1D gapped systems was proposed recently [95, 69, 33].

The thermal mixed state  $\exp(-H/T)$  ( $T$  is the temperature) of any local Hamiltonian  $H$  in any spatial dimension is well approximated by a projected entangled pair operator of bond dimension  $D = n^{O(1/T)}$  [104], where  $n$  is the system size. This result is built on the techniques developed in previous works [62, 93].

## 2.4 Area law

As a main object of study in this dissertation, the notion of “area law” [40] for entanglement has received much attention in the community. An area law states that for certain interesting classes of quantum many-body states, the amount of entanglement between a subsystem and its complement grows as the boundary (area) rather than the volume of the subsystem. Formally, suppose a quantum lattice system is partitioned into two regions  $L$  and  $\bar{L}$ . If a state satisfies an area law, then the amount of entanglement between  $L$  and  $\bar{L}$  is upper bounded by  $O(|\partial L|)$ . Note that we usually use the entanglement entropy, i.e., the von Neumann entropy of the reduced density matrix on  $L$ , as the measure of entanglement for pure quantum states.

Area law has its origins in black hole thermodynamics, cf. the holographic principle. It is of interest to condensed matter theorists because it characterizes the structure of entanglement in quantum many-body states. Indeed, a generic state satisfies a volume law rather than an area law [65]. Thus, area law provides a rigorous formulation of the statement that many physically relevant states are highly non-generic and only occupy a small corner of the entire Hilbert space.

Another important motivation to study area law is that it is related to the classical simulability of quantum many-body systems. In contrast to the fact that a generic state requires an exponential number of bits to describe, states that satisfy an area law are heuristically expected to allow efficient classical approximations using (e.g.) tensor network states of small bond dimension. Indeed, MPS in 1D and PEPS in 2+D are intentionally constructed to satisfy an area law: For any region  $L$ , the Schmidt rank between  $L$  and  $\bar{L}$  is upper bounded by  $D^{|\partial L|}$ , where  $D$  is the bond dimension. Hence, the entanglement entropy is upper bounded by  $|\partial L| \log D$ , giving rise to an area law if  $D$  is a constant. Furthermore, MPS or PEPS of polynomial bond dimension can at most describe states that violate area law by a logarithmic factor.

We now give some intuition on why it is reasonable to believe an area law in the ground states of gapped local Hamiltonians in any spatial dimension. Indeed, Hastings [60] proved that these ground states have exponential decay of correlations, e.g., any correlation functions decay exponentially with distance. Intuitively, exponential decay of correlations implies that the entanglement between a region and its complement is localized near the boundary (within a distance of the order of the correlation length). However, establishing this implication rigorously is very challenging. Note that the ground states of 1D local Hamiltonians with an inverse polynomial energy gap can have a volume law of entanglement [52] even in the presence of translational invariance [83].

Typically, proving area laws rigorously is very difficult. It was not until 2007 that Hastings proved [59] that the ground states of all 1D gapped Hamiltonians satisfy an area law (this is a breakthrough!). As a by-product, these ground states allow MPS approximations of polynomial bond dimension. Hastings’ proof uses the Lieb-Robinson bound [100] and the Fourier transform. Recently, Arad, Kitaev, Landau, and Vazirani [10] developed a combinatorial proof of the area law in 1D gapped systems. This proof significantly improves the upper bound of Hastings (on the entanglement entropy). Furthermore, it was adapted to

the setting of constant-fold degenerate ground states [70]. In particular, any state in the ground-state space satisfies an area law. Brandao and Horodecki [19, 18] showed that exponential decay of correlations implies an area law in 1D. Together with Hastings' result [60] that the ground states of gapped local Hamiltonians have exponential decay of correlations, we get another proof of 1D area law. The upper bound obtained in this way matches that of Hastings in [59].

However, it is easy to prove an area law for the thermal mixed state of any local Hamiltonian, regardless of the energy gap or the spatial dimension of the underlying lattice [165]. It is important to note that we cannot use the entanglement entropy because thermal states are not pure states. Instead, we use mutual information as a measure of correlation.

The most well-known open problem in this area is whether an area law holds for the ground states of all gapped Hamiltonians in any spatial dimension. Recently, it was proved that the ground state of a gapped local Hamiltonian satisfies an area law if and only if all other ground states in the same phase satisfy an area law [1].

## 2.5 Complexity of the local Hamiltonian problem

QMA is the notion that captures the computational complexity of the local Hamiltonian problem. Roughly speaking, it is the quantum (and probabilistic) analog of NP. The verifier uses a quantum computer instead of a classical computer, and the proof can be a quantum state. Since measurement outcomes in quantum mechanics are inherently random, the verifier should be allowed to err with small probability. Formally, we define QMA using quantum circuits as a quantum verifier.

**Definition 1** (QMA). A problem is in QMA if and only if there exists a uniform family of polynomial-size quantum circuits  $\{Q_x\}$  (one for each input instance  $x$ ) such that:

- 1 (completeness). If  $x$  is a yes instance, then there exists a quantum state  $|y\rangle$  of polynomial size such that  $Q_x$  accepts  $|y\rangle$  with probability at least  $2/3$ ;
- 2 (soundness). If  $x$  is a no instance, then for any quantum state  $|y\rangle$  of polynomial size,  $Q_x$  accepts  $|y\rangle$  with probability at most  $1/3$ .

We have set the error probability to be  $1/3$ . Indeed, this number is quite arbitrary and can be made exponentially small by applying the circuit  $Q_x$  many times in parallel to many copies of the proof  $|y\rangle$  [8], cf. a biased coin can be detected with high probability by tossing it many times.

Similar to NP, the complexity class QMA also has complete problems. The canonical example is the local Hamiltonian problem. Formally, a  $k$ -local Hamiltonian acting on  $n$  spins (each of which has local dimension  $d = \Theta(1)$ ) is a Hermitian operator  $H = \sum_i H_i$ , where each term  $H_i$  acts non-trivially on  $k$  spins.

Suppose every real number is represented by a polynomial number of bits.

**Definition 2** ( $k$ -local Hamiltonian problem [91]). We are given a  $k$ -local Hamiltonian  $H$  and a real number  $a$  with the promise that either (Yes)  $\lambda(H) \leq a$  or (No)  $\lambda(H) \geq a + \delta$ ,

where  $\lambda(H)$  denotes the ground-state energy (i.e., the smallest eigenvalue) of  $H$ , and  $\delta$  is some inverse polynomial in the system size. We must decide which is the case.

Apparently, the local Hamiltonian problem is a generalization of the satisfiability problem (a well-known NP-complete problem). Indeed, it is easy to construct a reduction from a satisfiability problem to a local Hamiltonian problem, where each term  $H_i$  is diagonal in the computational basis and encodes a constraint in the satisfiability problem by penalizing unsatisfying assignments. Then, a satisfying assignment corresponds to a product state with zero energy. This simple argument implies that the local Hamiltonian problem is NP-hard. We expect the local Hamiltonian problem to be much harder as it is QMA-complete.

We now briefly review known results on the computational complexity of the local Hamiltonian problem in various settings. Since this dissertation is mostly written for physicists, certain results that are of limited interest in physics will not be covered in detail, although they might be very interesting to computer scientists.

In a pioneering work, Kitaev [91] developed the quantum analog of the Cook-Levin theorem: The  $k$ -local Hamiltonian problem is in QMA for  $k \geq 1$  and QMA-hard for  $k \geq 5$ . Kitaev's proof is based on a combination of the ideas behind the Cook-Levin theorem and the early ideas of Feynman for a quantum computer [42]. Subsequently, the 3-local Hamiltonian problem was shown to be QMA-complete [86] (see [106] for an alternative proof), and Kempe, Kitaev, and Regev [85] proved that the 2-local Hamiltonian problem is QMA-complete. Note that the 1-local Hamiltonian problem is trivially in P.

From a physicist's perspective, however, the Hamiltonians involved in the aforementioned QMA-hardness proofs are not very physical in the sense that the particles (or spins) are not arranged on a regular lattice. To address this, Oliveira and Terhal [111] showed that the local Hamiltonian problem is QMA-complete even if it is restricted to a 2D square lattice with nearest-neighbor interactions. Subsequently, it was found that the 2D Heisenberg model in a nonuniform magnetic field is QMA-complete [137]. In contrast to the classical case of the satisfiability problem on a line (which can be easily solved in polynomial time by dynamic programming), Aharonov, Gottesman, Irani and Kempe [7] showed that the 1D local Hamiltonian problem with nearest-neighbor interactions is QMA-complete if the local dimension is at least 13. The local dimension can be reduced to 8 [58]. Gottesman and Irani [53] obtained similar results for translationally invariant 1D systems (see also [84]).

As a special case of the  $k$ -local Hamiltonian problem, one might ask whether a given  $k$ -local Hamiltonian is frustration-free, i.e., whether the ground state of the  $k$ -local Hamiltonian  $H = \sum_i H_i$  is the ground state of each individual term  $H_i$ . Bravyi [20] showed that the problem is in P for  $k = 2$ , and is QMA<sub>1</sub>-complete for  $k \geq 4$ , where QMA<sub>1</sub> is the variant of QMA with perfect completeness. Recently, Gosset and Nagaj [51] showed that the problem is also QMA<sub>1</sub>-complete for  $k = 3$ .

The second special case of local Hamiltonians is commuting local Hamiltonians, which are interesting to physicists because most exactly solvable models (e.g., the toric code) for topological order in 2+D are commuting (and frustration-free). It was shown the commuting 2-local Hamiltonian problem on qudits [24] and the commuting 3-local Hamiltonian problem

on qubits [4] are in NP. Furthermore, Ref. [4] showed that the toric code is in some rigorous sense the “minimal model” for topological order. In 1D, the ground states of commuting local Hamiltonians can be expressed exactly (up to the truncation of real numbers) as MPS of constant bond dimension, and the ground-state energy can be computed efficiently by dynamic programming [5, 135].

Another special case of local Hamiltonians is stoquastic local Hamiltonians, in which each individual term has only non-positive off-diagonal matrix elements in the computational basis. Stoquastic local Hamiltonians do not suffer from the so-called “sign problem” in quantum Monte Carlo simulations and thus are expected to be easier than general local Hamiltonians. Note that quantum Monte Carlo is not a quantum algorithm; it is just a classical Monte Carlo algorithm applied to quantum systems. See Refs. [21, 23] for results on the computational complexity of stoquastic local Hamiltonians.

The local Hamiltonian problem is QMA-complete for indistinguishable particles (both fermions [101] and bosons [160]). It is also QMA-complete for the 2D Hubbard model at half filling in a nonuniform magnetic field [137] and for the Bose-Hubbard model on general interaction graphs (i.e., not on a regular lattice) [32].

The PCP theorem is one of the cornerstones of modern complexity theory. Hence, a major open problem for computer scientists is whether a quantum analog of this theorem holds [8]. The quantum PCP conjecture is of limited interest in physics because it is apparently not true on a lattice. We refer interested readers to the recent survey [3] on this topic.

## Chapter 3

# Area law for degenerate ground states in one dimension

An area law is proved for the Renyi entanglement entropy of possibly degenerate ground states in 1D gapped quantum systems. Suppose in a chain of  $n$  spins the ground states of a local Hamiltonian with energy gap  $\epsilon$  are constant-fold degenerate. Then, the Renyi entanglement entropy  $R_\alpha(0 < \alpha < 1)$  of any ground state across any cut is upper bounded by  $\tilde{O}(\alpha^{-3}/\epsilon)$ , and any ground state can be well approximated by an MPS of sub-polynomial bond dimension  $2^{\tilde{O}(\epsilon^{-1/4} \log^{3/4} n)}$ .

### 3.1 Introduction

The area law states that for a large class of “physical” quantum many-body states the entanglement of a region scales as its boundary (area) [40]. This is in sharp contrast to the volume law for generic states [65]: the entanglement of a region scales as the number of sites in (i.e., the volume of) the region. In 1D, the area law is of particular interest for it characterizes the classical simulability of quantum systems. Specifically, bounded (or even logarithmic divergence of) Renyi entanglement entropy across all cuts implies efficient MPS representations [146], which underlie the (heuristic) DMRG algorithm [161, 162]. Since MPS can be efficiently contracted, the 1D local Hamiltonian problem with the restriction that the ground state satisfies area laws is in NP. Furthermore, a structural result from the proof of the area law for the ground state of 1D gapped Hamiltonians is an essential ingredient of the (provably) polynomial-time algorithm [95, 69, 33] for computing such states, establishing that the 1D gapped local Hamiltonian problem is in P. The area law is now a central topic in the emerging field of Hamiltonian complexity [113, 49].

We start with the definition of entanglement entropy.

**Definition 3** (Entanglement entropy). The Renyi entanglement entropy  $R_\alpha(0 < \alpha < 1)$  of

Table 3.1: Relations between various conditions in 1D: unique ground state of a gapped local Hamiltonian (Gap), exponential decay of correlations (Exp), area law for Renyi entanglement entropy  $R_\alpha, \forall \alpha$  (AL- $R_\alpha$ ), area law for von Neumann entanglement entropy (AL- $S$ ), efficient matrix product state representation (MPS). A check (cross) mark means that the item in the row implies (does not imply) the item in the column. The asterisk marks one contribution of this chapter. It is an open problem whether exponential decay of correlations implies area laws for Renyi entanglement entropy  $R_\alpha, \forall \alpha$ : Indeed, Theorem 4 in [19] (or Theorem 1 in [18]) may lead to divergence of  $R_\alpha$  if  $\alpha$  is small.

	Exp	AL- $R_\alpha$	AL- $S$	MPS
Gap	✓[60]	✓*	✓[59, 10]	✓[59, 10]
Exp	✓	?	✓[19, 18]	✓[19, 18]
AL- $R_\alpha$	X	✓	✓	✓[146]
AL- $S$	X	X	✓	X[139]

a bipartite (pure) quantum state  $\rho_{AB}$  is defined as

$$R_\alpha(\rho_A) = (1 - \alpha)^{-1} \log \text{tr} \rho_A^\alpha, \quad (3.1)$$

where  $\rho_A = \text{tr}_B \rho_{AB}$  is the reduced density matrix. The von Neumann entanglement entropy is defined as

$$S(\rho_A) = -\text{tr}(\rho_A \log \rho_A) = \lim_{\alpha \rightarrow 1^-} R_\alpha(\rho_A). \quad (3.2)$$

Here are three arguments why Renyi entanglement entropy is more suitable than von Neumann entanglement entropy for formulating area laws, although the latter is the most popular entanglement measure (for pure states) in quantum information and condensed matter theory.

1 (conceptual, classical simulability). In 1D, (unlike bounded Renyi entanglement entropy) bounded von Neumann entanglement entropy across all cuts does not necessarily imply efficient MPS representations; see [139] for a counterexample. Although slightly outside the scope of this chapter, related results are summarized in Table 3.1.

2 (conceptual, quantum computation). Quantum states with little von Neumann entanglement entropy across all cuts support universal quantum computation, while an analogous statement for Renyi entanglement entropy is expected to be false [145].

3 (technical). An area law for Renyi entanglement entropy implies that for von Neumann entanglement entropy, as  $R_\alpha$  is a monotonically decreasing function of  $\alpha$ .

Hastings first proved an area law for the ground state of 1D Hamiltonians with energy gap  $\epsilon$ : The von Neumann entanglement entropy across any cut is upper bounded by  $2^{O(\epsilon^{-1})}$  [59], where the local dimension of each spin (denoted by “ $d$ ” in qudits) is assumed to be an absolute constant. The Renyi entanglement entropy  $R_\alpha$  for  $\alpha_0 < \alpha < 1$  was also discussed, where  $\alpha_0$  is  $\epsilon$ -dependent and  $\lim_{\epsilon \rightarrow 0^+} \alpha_0 = 1$ . The bound on the von Neumann entanglement entropy was recently improved to  $\tilde{O}(\epsilon^{-3/2})$  [10] (see Section 3.5 for an explanation of this

result), where  $\tilde{O}(x) := O(x \text{ poly log } x)$  hides a polylogarithmic factor. These proofs of area laws assume a unique (non-degenerate) ground state.

Ground-state degeneracy is an important physical phenomenon often associated with symmetry breaking (e.g., the transverse field Ising chain) and/or topological order (e.g., the Haldane/AKLT chain with open boundary conditions). Since not all degenerate ground states of 1D gapped Hamiltonians have exponential decay of correlations, it may not be intuitively obvious to what extent they satisfy area laws.

In this chapter, an area law is proved for the Renyi entanglement entropy of possibly degenerate ground states in 1D gapped systems. Since in this context the standard bra-ket notation may be cumbersome, quantum states and their inner products are simply denoted by  $\psi, \phi \dots$  and  $\langle \psi, \phi \rangle$ , respectively, cf.  $\| |\psi\rangle - |\phi\rangle \|$  versus  $\| \psi - \phi \|$ . Suppose in a chain of  $n$  spins the ground states are constant-fold degenerate.

**Theorem 1.** (a) *The Renyi entanglement entropy  $R_\alpha(0 < \alpha < 1)$  of any ground state across any cut is upper bounded by  $\tilde{O}(\alpha^{-3}/\epsilon)$ ;*

(b) *Any ground state  $\psi$  can be approximated by an MPS  $\phi$  of sub-polynomial bond dimension  $2^{\tilde{O}(\epsilon^{-1/4} \log^{3/4} n)}$  such that  $|\langle \psi, \phi \rangle| > 1 - 1/\text{poly}(n)$ .*

*Remark.* The proof of this theorem assumes constant-fold exact ground-state degeneracy and open boundary conditions (with one cut). It should be clear that a minor modification of the proof leads to the same results in the presence of an exponentially small  $2^{-\Omega(n)}$  splitting of the ground-state degeneracy (as is typically observed in physical systems) and works for periodic boundary conditions (with two cuts). However, it remains an open problem to what extent degenerate ground states satisfy area laws if the degeneracy grows with the system size. Theorem 1(b) is a theoretical justification of the practical success of DMRG as a (heuristic) variational algorithm over MPS to compute the ground-state space in 1D gapped systems with ground-state degeneracy, and paves the way for a (provably) polynomial-time algorithm to compute the ground-state space [69, 33]. As an important immediate corollary of Theorem 1(a), the von Neumann entanglement entropy of a unique ground state is upper bounded by  $\tilde{O}(\epsilon^{-1})$ , which even improves the result of [10] and may possibly be tight up to a polylogarithmic factor. An example with the von Neumann entanglement entropy  $S = \tilde{\Omega}(\epsilon^{-1/4})$  was constructed in [52]; see also [83] for a translationally invariant construction with  $S = \Omega(\epsilon^{-1/12})$ .

We loosely follow the approach in [10] with additional technical ingredients. Approximate ground-space projection (AGSP) [12] is a tool for bounding the decay of Schmidt coefficients: An “efficient” family of AGSP imply an area law. Section 3.2 is devoted to perturbation theory, which is necessary to improve the efficiency of AGSP. As a technical contribution, the analysis in Section 6 of [10] is improved (and simplified), resulting in a tightened upper bound  $\tilde{O}(\epsilon^{-1})$  (versus  $\tilde{O}(\epsilon^{-3/2})$  given in [10]) on the (von Neumann) entanglement entropy. Although the perturbation theory is developed in 1D, generalizations to higher dimensions may be straightforward but are not presented in this chapter. In Section 3.3, a family of AGSP are constructed in 1D systems with nearly degenerate ground states. Although the



ground-state degeneracy of the original Hamiltonian is assumed to be exact, perturbations may lead to an exponentially small splitting of the degeneracy. Then, “fine tuning” using Lagrange interpolation polynomials appears necessary to repair this splitting at the level of AGSP. In Section 3.4, an area law is derived from AGSP for any ground state by constructing a sequence of approximations to a set of basis vectors of the ground-state space (it requires new ideas to keep track of such a set of basis vectors). The construction is more efficient than the approach (Corollary 2.4 and Section 6.2) in [10], resulting in an area law for the Renyi entanglement entropy. Finally, efficient MPS representations follow from the decay of the Schmidt coefficients.

## 3.2 Perturbation theory

Assume without loss of generality that the original 1D Hamiltonian is  $H' = \sum_{i=-n}^n H'_i$ , where  $0 \leq H'_i \leq 1$  acts on the spins  $i$  and  $i + 1$ . Consider the middle cut. Let  $\epsilon_0(\cdot)$  denote the ground-state energy of a Hamiltonian. Define

$$H = H_L + H_{-s} + H_{1-s} + \cdots + H_{s-1} + H_s + H_R \quad (3.3)$$

as

- (i)  $H_L = H'_L - \epsilon_0(H'_L)$  and  $H_R = H'_R - \epsilon_0(H'_R)$ , where  $H'_L := \sum_{i=-n}^{-s-1} H'_i$  and  $H'_R := \sum_{i=s+1}^n H'_i$ ;
- (ii)  $H_i = H'_i$  for  $i = \pm s$ ;
- (iii)  $H_i = H'_i - \epsilon_0(H'_M)/(2s - 1)$  for  $1 - s \leq i \leq s - 1$ , where  $H'_M := \sum_{i=1-s}^{s-1} H'_i$ .

Hence,

- (a)  $H_L \geq 0$ ,  $H_R \geq 0$ , and  $\epsilon_0(H_L) = \epsilon_0(H_R) = 0$ ;
- (b)  $0 \leq H_i \leq 1$  for  $i = \pm s$ ;
- (c)  $0 \leq \sum_{i=1-s}^{s-1} H_i \leq 2s - 1$  and  $\epsilon_0(\sum_{i=1-s}^{s-1} H_i) = 0$ ;
- (d)  $H = H' - \epsilon_0(H'_L) - \epsilon_0(H'_M) - \epsilon_0(H'_R)$  so that the (degenerate) ground states and the energy gap are preserved.

Suppose the ground states of  $H$  are  $f$ -fold degenerate, where  $f = \Theta(1)$  is assumed to be an absolute constant. Let  $0 \leq \epsilon_0 = \epsilon_1 = \cdots = \epsilon_{f-1} < \epsilon_f \leq \epsilon_{f+1} \leq \cdots$  be the lowest energy levels of  $H$  with the energy gap  $\epsilon := \epsilon_f - \epsilon_0$ . Define

$$H_L^{\leq t} = H_L P_L^{\leq t} + t(1 - P_L^{\leq t}), \quad (3.4)$$

where  $P_L^{\leq t}$  is the projection onto the subspace spanned by the eigenstates of  $H_L$  with eigenvalues at most  $t$ .  $H_R^{\leq t}$  is defined analogously. Let

$$H^{(t)} := H_L^{\leq t} + H_{-s} + H_{1-s} + \cdots + H_{s-1} + H_s + H_R^{\leq t} \leq 2t + 2s + 1 \quad (3.5)$$

be the truncated Hamiltonian with the lowest energy levels  $0 \leq \epsilon'_0 \leq \epsilon'_1 \leq \cdots$  and the corresponding (orthonormal) eigenstates  $\phi_0^{(t)}, \phi_1^{(t)}, \dots$ . Note that all states are normalized unless otherwise stated. Define  $\epsilon' = \epsilon'_f - \epsilon'_0$  as the energy gap of  $H^{(t)}$ . Let  $B := H_{-s} + H_s$

be the sum of boundary terms, and  $P_t$  be the projection onto the subspace spanned by the eigenstates of  $H - B$  with eigenvalues at most  $t$  so that

$$H_L P_t = H_L^{\leq t} P_t, H_R P_t = H_R^{\leq t} P_t \Rightarrow H P_t = H^{(t)} P_t. \quad (3.6)$$

**Lemma 1.**  $0 \leq \epsilon'_0 \leq \epsilon_0 \leq 2$  and  $\epsilon'_f \leq \epsilon_f \leq [\log_2 f] + 4 = O(1)$ .

*Proof.* Let  $\psi_0, \psi_L, \psi_M, \psi_R$  be the ground states of  $H, H_L, \sum_{i=1-s}^{s-1} H_i, H_R$ , respectively.

$$\begin{aligned} \epsilon_0 &\leq \langle \psi_L \psi_M \psi_R, H \psi_L \psi_M \psi_R \rangle \\ &= \langle \psi_L, H_L \psi_L \rangle + \left\langle \psi_M, \sum_{i=1-s}^{s-1} H_i \psi_M \right\rangle + \langle \psi_R, H_R \psi_R \rangle + \langle \psi_L \psi_M \psi_R, B \psi_L \psi_M \psi_R \rangle \\ &\leq \|B\| \leq 2. \end{aligned} \quad (3.7)$$

Let  $f' = [\log_2 f] + 1$  and  $\phi_R$  be the ground state of  $\sum_{i=f'-s+1}^s H_i + H_R$ . For any state  $\phi_M$  of the spins  $1-s, 2-s, \dots, f'-s$ ,

$$\begin{aligned} &\langle \psi_L \phi_M \phi_R, H \psi_L \phi_M \phi_R \rangle \\ &= \langle \psi_L, H_L \psi_L \rangle + \left\langle \psi_L \phi_M \phi_R, \sum_{i=-s}^{f'-s} H_i \psi_L \phi_M \phi_R \right\rangle + \left\langle \phi_R, \left( \sum_{i=f'+1-s}^s H_i + H_R \right) \phi_R \right\rangle \\ &\leq \langle \psi, H_L \psi \rangle + \left\langle \psi, \sum_{i=-s}^{f'-s} H_i \psi \right\rangle + f' + 1 + \left\langle \psi, \left( \sum_{i=f'+1-s}^s H_i + H_R \right) \psi \right\rangle \\ &\leq \langle \psi, H \psi \rangle + f' + 1 = \epsilon_0 + f' + 1 \leq f' + 3 \Rightarrow \epsilon_f \leq f' + 3 = [\log_2 f] + 4. \end{aligned} \quad (3.8)$$

□

Let  $\phi^{(r)}$  be an eigenstate of  $H^{(r)}$  with eigenvalue  $\epsilon^{(r)}$ .

**Lemma 2.** For  $r, t > \epsilon^{(r)}$ ,

$$\|(1 - P_t) \phi^{(r)}\|^2 \leq |\langle \phi^{(r)}, (1 - P_t) B P_t \phi^{(r)} \rangle| / (\min\{r, t\} - \epsilon^{(r)}). \quad (3.9)$$

*Proof.* It follows from

$$\begin{aligned} \epsilon^{(r)} &= \langle \phi^{(r)}, H^{(r)} \phi^{(r)} \rangle \\ &= \langle \phi^{(r)}, (1 - P_t) H^{(r)} (1 - P_t) \phi^{(r)} \rangle + \langle \phi^{(r)}, P_t H^{(r)} \phi^{(r)} \rangle + \langle \phi^{(r)}, (1 - P_t) H^{(r)} P_t \phi^{(r)} \rangle \\ &\geq \langle \phi^{(r)}, (1 - P_t) (H^{(r)} - B) (1 - P_t) \phi^{(r)} \rangle + \epsilon^{(r)} \|P_t \phi^{(r)}\|^2 \\ &\quad + \langle \phi^{(r)}, (1 - P_t) (H^{(r)} - B) P_t \phi^{(r)} \rangle + \langle \phi^{(r)}, (1 - P_t) B P_t \phi^{(r)} \rangle \\ &\geq \min\{r, t\} \|(1 - P_t) \phi^{(r)}\|^2 + \epsilon^{(r)} (1 - \|(1 - P_t) \phi^{(r)}\|^2) \\ &\quad - |\langle \phi^{(r)}, (1 - P_t) B P_t \phi^{(r)} \rangle|. \end{aligned} \quad (3.10)$$

□

Suppose  $\epsilon^{(r)} = O(1)$  and  $r \geq \epsilon^{(r)} + 100 = O(1)$ .

**Lemma 3.**

$$\|(1 - P_t)\phi^{(r)}\| \leq 2^{-\Omega(t)}. \quad (3.11)$$

*Proof.* Let  $t_0 = \epsilon^{(r)} + 100 = O(1)$ . We show that there exists  $c = O(1)$  such that

$$\|(1 - P_{t_i})\phi^{(r)}\| \leq 2^{-i} \quad (3.12)$$

for  $t_i = t_0 + ci$ . The proof is an induction on  $i$  with fixed  $r$ . Clearly, (3.12) holds for  $i = 0$ . Suppose it holds for  $i = 0, 1, \dots, j-1$ . Let  $P_{t_{-1}} = 0$  for notational convenience. Lemma 2 implies

$$\begin{aligned} \|(1 - P_{t_j})\phi^{(r)}\|^2 &\leq |\langle \phi^{(r)}, (1 - P_{t_j})BP_{t_j}\phi^{(r)} \rangle| / (\min\{r, t_j\} - \epsilon^{(r)}) \\ &\leq \left| \left\langle \phi^{(r)}, (1 - P_{t_j})B \sum_{i=0}^j (P_{t_i} - P_{t_{i-1}})\phi^{(r)} \right\rangle \right| / 100 \\ &\leq \|(1 - P_{t_j})\phi^{(r)}\| \sum_{i=0}^j \|(1 - P_{t_j})B(P_{t_i} - P_{t_{i-1}})\| \|(P_{t_i} - P_{t_{i-1}})\phi^{(r)}\| / 100 \\ &\Rightarrow \|(1 - P_{t_j})\phi^{(r)}\| \leq \sum_{i=0}^j \|(1 - P_{t_j})BP_{t_i}\| \|(1 - P_{t_{i-1}})\phi^{(r)}\| / 100 \\ &\leq \sum_{i=0}^j e^{(t_i - t_j)/8} 2^{-i} / 10, \end{aligned} \quad (3.13)$$

where we have used the induction hypothesis and the inequality  $\|(1 - P_{t_j})BP_{t_i}\| \leq 4e^{(t_i - t_j)/8}$  (Lemma 6.6(2) in [10]). Hence (3.12) holds for  $i = j$  by setting  $c = 16 \ln 2$ .  $\square$

Let  $\Phi^{(t)} := P_t\phi^{(t)} / \|P_t\phi^{(t)}\|$ .

**Lemma 4.**

$$\langle \Phi^{(t)}, H\Phi^{(t)} \rangle \leq \epsilon^{(t)} + 2^{-\Omega(t)}. \quad (3.14)$$

*Proof.* (3.6) implies

$$\begin{aligned} \epsilon^{(t)} &= \langle \phi^{(t)}, H^{(t)}\phi^{(t)} \rangle \\ &\geq \langle \phi^{(t)}, P_t H^{(t)} P_t \phi^{(t)} \rangle + \langle \phi^{(t)}, P_t H^{(t)} (1 - P_t)\phi^{(t)} \rangle + \langle \phi^{(t)}, (1 - P_t) H^{(t)} P_t \phi^{(t)} \rangle \\ &= \langle \phi^{(t)}, P_t H P_t \phi^{(t)} \rangle + \langle \phi^{(t)}, P_t B (1 - P_t)\phi^{(t)} \rangle + \langle \phi^{(t)}, (1 - P_t) B P_t \phi^{(t)} \rangle \\ &\geq \langle \phi^{(t)}, P_t H P_t \phi^{(t)} \rangle - 2\|BP_t\phi^{(t)}\| \cdot \|(1 - P_t)\phi^{(t)}\| \geq \langle \phi^{(t)}, P_t H P_t \phi^{(t)} \rangle - 2^{-\Omega(t)} \\ &\Rightarrow \langle \Phi^{(t)}, H\Phi^{(t)} \rangle \leq (\epsilon^{(t)} + 2^{-\Omega(t)}) / \|P_t\phi^{(t)}\|^2 \\ &= (\epsilon^{(t)} + 2^{-\Omega(t)}) / (1 - 2^{-\Omega(t)}) = \epsilon^{(t)} + 2^{-\Omega(t)}. \end{aligned} \quad (3.15)$$

$\square$

*Remark.* Suppose  $r \geq t$ . A very minor modification of the proof implies

$$\langle \Phi^{(r),t}, H\Phi^{(r),t} \rangle \leq \epsilon^{(r)} + 2^{-\Omega(t)} \text{ for } \Phi^{(r),t} := P_t \phi^{(r)} / \|P_t \phi^{(r)}\|. \quad (3.16)$$

Since the proofs of Lemmas 1–4 do not require an energy gap, these lemmas also hold in gapless systems. Let  $G$  be the ground-state space of  $H$ .

**Lemma 5.** *For any state  $\psi$  with  $\langle \psi, H\psi \rangle \leq \epsilon_0 + \epsilon$ , there exists a state  $\psi_g \in G$  such that*

$$\|\psi - \psi_g\|^2 \leq 2\epsilon/\epsilon. \quad (3.17)$$

*Proof.* The state  $\psi$  can be decomposed as

$$\psi = c_g \psi_g + c_e \psi_e, \quad c_g, c_e \geq 0, \quad c_g^2 + c_e^2 = 1, \quad (3.18)$$

where  $\psi_g \in G$  and  $\psi_e \perp G$ . Then,

$$c_g^2 \epsilon_0 + c_e^2 \epsilon_f \leq \langle \psi, H\psi \rangle \leq \epsilon_0 + \epsilon \Rightarrow c_e^2 \leq \epsilon/\epsilon \Rightarrow \|\psi - \psi_g\|^2 = 2 - 2c_g \leq 2\epsilon/\epsilon. \quad (3.19)$$

□

**Theorem 2.** *For  $t \geq O(\log \epsilon^{-1})$ ,*

(a)  $0 \leq \epsilon_0 - \epsilon'_{f-1} \leq \epsilon_0 - \epsilon'_{f-2} \leq \dots \leq \epsilon_0 - \epsilon'_0 \leq 2^{-\Omega(t)}$ ;

(b) *there exists  $\psi_i^{(t)} \in G$  such that  $\|\psi_i^{(t)} - \phi_i^{(t)}\|^2 \leq 2^{-\Omega(t)}$  for  $i = 0, 1, \dots, f-1$ ;*

(c)  $\epsilon' \geq \epsilon/10$ .

*Proof.* Lemma 4 implies

$$\epsilon'_0 \leq \epsilon'_1 \leq \dots \leq \epsilon'_{f-1} \leq \epsilon_0 \leq \langle \Phi_0^{(t)}, H\Phi_0^{(t)} \rangle \leq \epsilon'_0 + 2^{-\Omega(t)}, \quad (3.20)$$

$$\langle \Phi_f^{(t)}, H\Phi_f^{(t)} \rangle \leq \epsilon'_f + 2^{-\Omega(t)} = \epsilon'_0 + \epsilon' + 2^{-\Omega(t)} \leq \epsilon_0 + \epsilon' + 2^{-\Omega(t)}. \quad (3.21)$$

(a) follows from (3.20). Using Lemma 5, there exists  $\psi_0^{(t)}, \psi_1^{(t)}, \dots, \psi_f^{(t)} \in G$  such that

$$\|\Phi_i^{(t)} - \psi_i^{(t)}\|^2 \leq 2^{-\Omega(t)}/\epsilon = 2^{-\Omega(t)+\log \epsilon^{-1}} \quad (3.22)$$

for  $i = 0, 1, \dots, f-1$  and

$$\|\Phi_f^{(t)} - \psi_f^{(t)}\|^2 \leq \epsilon'/\epsilon + 2^{-\Omega(t)}/\epsilon. \quad (3.23)$$

Lemma 3 implies

$$\|\phi_i^{(t)} - \Phi_i^{(t)}\|^2 \leq 2^{-\Omega(t)}. \quad (3.24)$$

(b) follows from (3.22), (3.24) as  $t \geq O(\log \epsilon^{-1})$ . (c) follows from (3.22), (3.23), (3.24), because  $\phi_0^{(t)}, \phi_1^{(t)}, \dots, \phi_f^{(t)}$  are pairwise orthogonal while  $\psi_0^{(t)}, \psi_1^{(t)}, \dots, \psi_f^{(t)}$  are linearly dependent. □

### 3.3 Approximate ground-space projection

Recall that  $H^{(t)}$  is the truncated Hamiltonian with the lowest energy levels  $0 \leq \epsilon'_0 \leq \epsilon'_1 \leq \dots$  and the corresponding (orthonormal) eigenstates  $\phi_0^{(t)}, \phi_1^{(t)}, \dots$ . Theorem 2 implies that the lowest  $f$  energy levels are nearly degenerate:  $\epsilon'_0 \approx \epsilon'_{f-1}$ , and  $\epsilon' = \epsilon'_f - \epsilon'_0$  is the energy gap. Let  $G' := \text{span}\{\phi_i^{(t)} | i = 0, 1, \dots, f-1\}$  be the ground-state space of  $H^{(t)}$ . Let  $R(\psi)$  denote the Schmidt rank of a state  $\psi$  across the middle cut.

**Definition 4** (Approximate ground-space projection (AGSP) [12]). A linear operator  $A$  is a  $(\Delta, D)$ -AGSP if

- (i)  $A\psi = \psi$  for  $\forall \psi \in G'$ ;
- (ii)  $A\psi \perp G'$  and  $\|A\psi\|^2 \leq \Delta$  for  $\forall \psi \perp G'$ ;
- (iii)  $R(A\psi) \leq DR(\psi)$  for  $\forall \psi$ .

Let  $\epsilon'_\infty := 2s + 2t + 1$  be an upper bound on the maximum eigenvalue of  $H^{(t)}$ .

**Lemma 6.** *Suppose  $l^2(\epsilon'_{f-1} - \epsilon'_0)/(\epsilon'_\infty - \epsilon'_f) \leq 1/10$ . Then there exists a polynomial  $C_l$  of degree  $fl$  such that*

- (i)  $C_l(\epsilon'_0) = C(\epsilon'_1) = \dots = C(\epsilon'_{f-1}) = 1$ ;
- (ii)  $C_l^2(x) \leq 2^{2f+4}e^{-4l\sqrt{\epsilon'/\epsilon'_\infty}}$  for  $\epsilon'_f \leq x \leq \epsilon'_\infty$ .

*Proof.* The Chebyshev polynomial of the first kind of degree  $l$  is defined as

$$T_l(x) = \cos(l \arccos x) = \cosh(ly), \quad y := \text{arccosh} x. \quad (3.25)$$

By definition,  $|T_l(x)| \leq 1$  for  $|x| \leq 1$ . For  $x \geq 1$ ,  $T_l(x)$  is monotonically increasing function of  $x$ , and

$$T_l(x) \geq e^{ly}/2 \geq e^{2l \tanh(y/2)}/2 = e^{2l\sqrt{(x-1)/(x+1)}}/2, \quad \frac{T'_l(x)}{T_l(x)} = \frac{l \tanh(ly)}{\sinh y} \leq \frac{l(ly)}{y} = l^2. \quad (3.26)$$

Let  $g(x) := (\epsilon'_\infty + \epsilon'_f - 2x)/(\epsilon'_\infty - \epsilon'_f)$  such that  $g(\epsilon'_\infty) = -1$  and  $g(\epsilon'_f) = 1$ . Define  $S_l(x) = T_l(g(x))$  as a polynomial of degree  $l$ . Clearly,  $|S_l(x)| \leq 1$  for  $\epsilon'_f \leq x \leq \epsilon'_\infty$  and

$$S_l(\epsilon'_0) = T_l(g(\epsilon'_0)) \geq e^{2l\sqrt{(g(\epsilon'_0)-1)/(g(\epsilon'_0)+1)}}/2 \geq e^{2l\sqrt{\epsilon'/\epsilon'_\infty}}/2. \quad (3.27)$$

There exists  $\epsilon'_0 \leq \xi \leq \epsilon'_{f-1}$  such that

$$\begin{aligned} S_l(\epsilon'_{f-1}) &= S_l(\epsilon'_0) + (\epsilon'_{f-1} - \epsilon'_0)S'_l(\xi) \geq S_l(\epsilon'_0)(1 + (\epsilon'_{f-1} - \epsilon'_0)T'_l(g(\xi))g'(\xi)/T_l(g(\xi))) \\ \Rightarrow S_l(\epsilon'_{f-1})/S_l(\epsilon'_0) &\geq 1 - 2l^2(\epsilon'_{f-1} - \epsilon'_0)/(\epsilon'_\infty - \epsilon'_f) \geq 4/5. \end{aligned} \quad (3.28)$$

Assume without loss of generality that  $\epsilon'_0, \epsilon'_1, \dots, \epsilon'_{f-1}$  are pairwise distinct. Let  $L(x) = \sum_{i=1}^f a_i x^i$  be the Lagrange interpolation polynomial of degree  $f$  such that  $L(0) = 0$  and

$L(S_l(\epsilon'_0)) = L(S_l(\epsilon'_1)) = \dots = L(S_l(\epsilon'_{f-1})) = S_l(\epsilon'_0)$ . For each  $i = 1, 2, \dots, f-1$ , there exists  $S_l(\epsilon'_{i-1}) > \xi_i > S_l(\epsilon'_i)$  such that  $L'(\xi_i) = 0$ . Then,

$$L'(x) = a_1 \prod_{i=1}^{f-1} (1 - x/\xi_i). \quad (3.29)$$

Clearly,  $a_1 > 0$  and  $L'(x) > 0$  for  $x < S_l(\epsilon'_{f-1})$ . Hence,

$$\begin{aligned} S_l(\epsilon'_0) &= L(S_l(\epsilon'_{f-1})) = \int_0^{S_l(\epsilon'_{f-1})} L'(x) dx \geq a_1 \int_0^{S_l(\epsilon'_{f-1})} (1 - x/S_l(\epsilon'_{f-1}))^{f-1} dx \\ &= a_1 S_l(\epsilon'_{f-1})/f \Rightarrow a_1 \leq 5f/4. \end{aligned} \quad (3.30)$$

For  $|x| \leq 1$ ,

$$\xi_1 > \xi_2 > \dots > \xi_{f-1} > S_l(\epsilon'_f) = 1 \Rightarrow |L'(x)| \leq a_1(1 + |x|)^{f-1} \Rightarrow |L(x)| \leq 2^{f+1}. \quad (3.31)$$

Finally,  $C_l(x) := L(S_l(x))/S_l(\epsilon'_0)$  is a polynomial of degree  $fl$ .  $\square$

**Lemma 7** (Lemma 4.2 in [10]). *For any polynomial  $p_l$  of degree  $l \leq s^2$  and any  $t, \psi$ ,*

$$R(p_l(H^{(t)})\psi) \leq l^{O(\sqrt{l})} R(\psi). \quad (3.32)$$

Let  $l = s^2/f$  and  $t = \Omega(s)$ . The assumption

$$1/10 \geq l^2(\epsilon'_{f-1} - \epsilon'_0)/(\epsilon'_\infty - \epsilon'_f) = O(s^4 2^{-\Omega(t)})/(s+t) = O(s^3 2^{-\Omega(s)}) \quad (3.33)$$

is satisfied with sufficiently large  $s > O(1)$ . Lemmas 6, 7 imply a  $(\Delta, D)$ -AGSP  $A = C_l(H^{(t)})$  for  $H^{(t)}$  with

$$\Delta = 2^{2f+4} e^{-4l\sqrt{\epsilon'/\epsilon'_\infty}} = 2^{-\Omega(s^2\sqrt{\epsilon'/t})}, \quad D = (s^2)^{O(\sqrt{s^2})} = s^{O(s)}. \quad (3.34)$$

In particular, the condition

$$1/100 \geq \Delta D^2 = 2^{-\Omega(s^2\sqrt{\epsilon'/t})} s^{O(s)} \Rightarrow 1/100 \geq \Delta D \quad (3.35)$$

can be satisfied by fixing  $t = t_0 = \Theta(s_0)$  and  $s = s_0 = \tilde{O}(\epsilon^{-1})$  so that  $\Delta = 2^{-\tilde{\Omega}(\epsilon^{-1})}$  and  $D = 2^{\tilde{O}(\epsilon^{-1})}$ .

### 3.4 Area law

Hereafter  $f = 2$  is assumed for ease of presentation. It should be clear that a very minor modification of the proof works for any  $f = O(1)$ . Suppose  $s = s_0$  and  $t = t_0$  as given above so that  $A$  is a  $(\Delta, D)$ -AGSP for  $H^{(t_0)}$  with  $\Delta D^2 \leq 1/100$ . Recall that  $\phi_0^{(t_0)}, \phi_1^{(t_0)}$  are the lowest two eigenstates and  $G' = \text{span}\{\phi_0^{(t_0)}, \phi_1^{(t_0)}\}$  is the ground-state space of  $H^{(t_0)}$ .

**Lemma 8.** *There exist  $\varphi_0, \varphi_1 \in G'$  and  $\psi_0, \psi'_0$  such that (i)  $\varphi_0 \perp \varphi_1$ ; (ii)  $|\langle \varphi_0, \psi_0 \rangle|^2 \geq 24/25$ ; (iii)  $R(\psi_0) = 2^{\tilde{O}(\epsilon^{-1})}$ ; (iv)  $|\langle \varphi_1, \psi'_0 \rangle|^2 \geq 24/25$ ; (v)  $R(\psi'_0) = 2^{\tilde{O}(\epsilon^{-1})}$ .*

*Proof.* Let  $P'$  be the projection onto  $G'$ . Consider

$$\max_{R(\psi)=1} \|P'\psi\|^2. \quad (3.36)$$

As the set  $\{\psi | R(\psi) = 1\}$  of product states is compact, the optimal state exists and is still denoted by  $\psi$ . This state and  $\phi := A\psi$  can be decomposed as

$$\psi = c_g \psi_g + c_e \psi_e, \quad \phi = c'_g \phi_g + c'_e \phi_e, \quad (3.37)$$

where  $\psi_g, \phi_g \in G'$  and  $\psi_e, \phi_e \perp G'$ . The definition of AGSP implies

$$c_g = c'_g, \quad \psi_g = \phi_g, \quad |c'_e|^2 \leq \Delta, \quad R(\phi) \leq D. \quad (3.38)$$

The Schmidt decomposition of the unnormalized state  $\phi$  implies

$$\phi = \sum_{i=1}^{R(\phi)} \lambda_i L_i \otimes R_i \Rightarrow \sum_{i=1}^{R(\phi)} \lambda_i^2 = \|\phi\|^2 = |c'_g|^2 + |c'_e|^2 \leq |c_g|^2 + \Delta. \quad (3.39)$$

Since  $|c_g|^2$  is the optimal value in (3.36),

$$\begin{aligned} |c_g| &= |\langle \psi_g, \phi \rangle| \leq \sum_{i=1}^{R(\phi)} \lambda_i |\langle \psi_g, L_i \otimes R_i \rangle| \leq \sum_{i=1}^{R(\phi)} \lambda_i \|P' L_i \otimes R_i\| \leq |c_g| \sum_{i=1}^{R(\phi)} \lambda_i \\ \Rightarrow 1 &\leq \left( \sum_{i=1}^{R(\phi)} \lambda_i \right)^2 \leq R(\phi) \sum_{i=1}^{R(\phi)} \lambda_i^2 \leq D(|c_g|^2 + \Delta) \leq D|c_g|^2 + 1/100 \\ \Rightarrow |c_g|^2 &\geq 99D^{-1}/100 \geq 99\Delta. \end{aligned} \quad (3.40)$$

Applying the AGSP twice, the state  $\psi_0 := A^2\psi/\|A^2\psi\|$  satisfies

$$\|P'\psi_0\|^2 \geq 1 - \Delta/50, \quad R(\psi_0) = D^2 = 2^{\tilde{O}(\epsilon^{-1})}. \quad (3.41)$$

Define  $\varphi_0 = P'\psi_0/\|P'\psi_0\| \in G'$  and  $\varphi_1 \in G'$  such that  $\varphi_0 \perp \varphi_1$ . Clearly,

$$|\langle \varphi_0, \psi_0 \rangle|^2 \geq 1 - \Delta/50, \quad \langle \varphi_1, \psi_0 \rangle = 0, \quad |\langle \varphi_e, \psi_0 \rangle|^2 \leq \Delta/50 \text{ for } \forall \varphi_e \perp G'. \quad (3.42)$$

Consider

$$\max_{R(\psi')=1} |\langle \varphi_1, \psi' \rangle|^2. \quad (3.43)$$

As the set  $\{\psi' | R(\psi') = 1\}$  of product states is compact, the optimal state exists and is still denoted by  $\psi'$ . This state and  $\phi' := A\psi' - \langle \psi_0, \psi' \rangle \psi_0$  can be decomposed as

$$\psi' = c_0 \varphi_0 + c_1 \varphi_1 + c_e \varphi_e, \quad \phi' = c_1 \varphi_1 + c_r \varphi_r, \quad (3.44)$$

where  $\varphi_e \perp G'$  and  $\varphi_r \perp \varphi_1$ . Specifically,

$$c_r \varphi_r = c_0(A\varphi_0 - \langle \psi_0, \varphi_0 \rangle \psi_0) - c_1 \langle \psi_0, \varphi_1 \rangle \psi_0 + c_e(A\varphi_e - \langle \psi_0, \varphi_e \rangle \psi_0) \quad (3.45)$$

implies

$$|c_r| \leq 0.2|c_0|\sqrt{\Delta} + 1.2|c_e|\sqrt{\Delta} \leq 1.4\sqrt{\Delta} \text{ and } R(\phi') \leq D + R(\psi_0) \leq D + D^2 \leq 2D^2. \quad (3.46)$$

The Schmidt decomposition of the unnormalized state  $\phi'$  implies

$$\phi' = \sum_{i=1}^{R(\phi')} \lambda'_i L'_i \otimes R'_i \Rightarrow \sum_{i=1}^{R(\phi')} \lambda_i'^2 = \|\phi'\|^2 = |c_1|^2 + |c_r|^2 \leq |c_1|^2 + 2\Delta. \quad (3.47)$$

Since  $\psi'$  is the optimal state,

$$\begin{aligned} |c_1| &= |\langle \varphi_1, \phi' \rangle| \leq \sum_{i=1}^{R(\phi')} \lambda'_i |\langle \varphi_1, L'_i \otimes R'_i \rangle| \leq \sum_{i=1}^{R(\phi')} \lambda'_i |\langle \varphi_1, \psi' \rangle| = |c_1| \sum_{i=1}^{R(\phi')} \lambda'_i \\ \Rightarrow 1 &\leq \left( \sum_{i=1}^{R(\phi')} \lambda'_i \right)^2 \leq R(\phi') \sum_{i=1}^{R(\phi')} \lambda_i'^2 \leq 2D^2(|c_1|^2 + 2\Delta) \leq 2D^2|c_1|^2 + 1/25 \\ \Rightarrow |c_1|^2 &\geq 12D^{-2}/25 \geq 48\Delta. \end{aligned} \quad (3.48)$$

Hence  $\psi'_0 = \phi'/\|\phi'\|$  is a state with  $R(\psi'_0) = R(\phi') \leq 2D^2 = 2\tilde{O}(\epsilon^{-1})$  and  $|\langle \varphi_1, \psi'_0 \rangle|^2 \geq 24/25$ .  $\square$

Recall that  $G$  is the ground-state space of  $H$ .

**Lemma 9.** *For any  $\Psi \in G$ , there is a sequence of approximations  $\{\Psi_i\}$  such that*

- (a)  $|\langle \Psi_i, \Psi \rangle| \geq 1 - 2^{-\Omega(i)}$ ;
- (b)  $R_i := R(\Psi_i) = 2^{\tilde{O}(\epsilon^{-1} + \epsilon^{-1/4} i^{3/4})}$ .

*Proof.* Let  $t_i = t_0 + i$ . Theorem 2(b) is a quantitative statement that  $G$  and  $\text{span}\{\phi_0^{(t_i)}, \phi_1^{(t_i)}\}$  are exponentially close. In particular, setting  $t_0$  to be a sufficiently large constant implies that  $G'$  and  $\text{span}\{\phi_0^{(t_i)}, \phi_1^{(t_i)}\}$  are close up to a small constant. Hence Lemma 8(ii) implies

$$|\langle \phi_0^{(t_i)}, \psi_0 \rangle|^2 + |\langle \phi_1^{(t_i)}, \psi_0 \rangle|^2 \geq 9/10. \quad (3.49)$$

Let  $l_i = s_i^2/2 = \Theta(\sqrt{t_i^3/\epsilon}) = O(t_i^2)$  such that the assumption

$$1/10 \geq l_i^2(\epsilon'_1 - \epsilon'_0)/(\epsilon'_\infty - \epsilon'_2) = O(s_i^3 2^{-\Omega(s_i)}) \quad (3.50)$$

is satisfied with sufficiently large  $s_i > O(1)$ . Lemmas 6, 7 imply a  $(\Delta_i, D_i)$ -AGSP  $A_i = C_{l_i}(H^{(t_i)})$  for  $H^{(t_i)}$  with

$$\Delta_i = 2^{-\Omega(s_i^2 \sqrt{\epsilon/t_i})} = 2^{-\Omega(t_i)}, \quad D_i = s_i^{O(s_i)} = 2^{\tilde{O}(\epsilon^{-1/4} i^{3/4})}. \quad (3.51)$$



Hence the sequence of operators  $\{A_i\}_{i=1}^{+\infty}$  converges exponentially due to Theorem 2(b). Clearly,  $A_\infty := \lim_{i \rightarrow +\infty} A_i$  is just the projection onto  $G$ . Let  $\psi_i := A_i \psi_0 / \|A_i \psi_0\|$  with  $\psi_\infty \in G$  such that

$$R(\psi_i) \leq R(\psi_0) D_i \leq 2^{\tilde{O}(\epsilon^{-1} + \epsilon^{-1/4} t_i^{3/4})}, \quad |\langle \psi_i, \psi_\infty \rangle| \geq 1 - 2^{-\Omega(t_i)}. \quad (3.52)$$

Similarly, Let  $\psi'_i := A_i \psi'_0 / \|A_i \psi'_0\|$  with  $\psi'_\infty \in G$  such that

$$R(\psi'_i) \leq 2^{\tilde{O}(\epsilon^{-1} + \epsilon^{-1/4} t_i^{3/4})}, \quad |\langle \psi'_i, \psi'_\infty \rangle| \geq 1 - 2^{-\Omega(t_i)}. \quad (3.53)$$

(3.49) with  $i = +\infty$  is a quantitative statement that  $\psi_0$  is close to  $G$ , and hence  $\psi_0$  and  $\psi_\infty$  are close up to a small constant. Since  $\psi_0$  and  $\varphi_0$  are close up to a small constant,  $\psi_\infty$  and  $\varphi_0$  are also close. The same arguments imply that  $\psi'_\infty$  and  $\varphi_1$  are close. Hence,  $\psi_\infty$  and  $\psi'_\infty$  are almost orthogonal. Any state  $\Psi \in G$  can be decomposed as

$$\Psi = c\psi_\infty + c'\psi'_\infty, \quad |c| = O(1), \quad |c'| = O(1). \quad (3.54)$$

Then,  $\{\Psi_i := c\psi_i + c'\psi'_i\}_{i=0}^{+\infty}$  is a sequence of approximations to  $\Psi$  with (b)  $R(\Psi_i) = 2^{\tilde{O}(\epsilon^{-1} + \epsilon^{-1/4} t_i^{3/4})}$ . (a) also follows immediately.  $\square$

*Proof of Theorem 1.* (a) Let  $\Lambda_i$  be the Schmidt coefficients of  $\Psi$  across the middle cut. Then,

$$1 - p_i := \sum_{j=1}^{R_i} \Lambda_j^2 \geq |\langle \Psi_i, \Psi \rangle|^2 \geq 1 - 2^{-\Omega(i)}. \quad (3.55)$$

The Renyi entanglement entropy of  $\Psi$  is upper bounded by

$$\begin{aligned} & \frac{\log \left( R_0^{1-\alpha} + \sum_{i=0}^{+\infty} p_i^\alpha (R_{i+1} - R_i)^{1-\alpha} \right)}{1-\alpha} \\ & \leq \frac{\log \left( 2^{(1-\alpha)\tilde{O}(\epsilon^{-1})} + \sum_{i=0}^{+\infty} 2^{(1-\alpha)\tilde{O}(\epsilon^{-1} + \epsilon^{-1/4} i^{3/4}) - \alpha\Omega(i)} \right)}{1-\alpha} \\ & = \tilde{O}(\epsilon^{-1}) + \frac{\log(O(1) + 2^{(1-\alpha)\tilde{O}((1-\alpha)^3\alpha^{-3}/\epsilon)})}{1-\alpha} \\ & = \tilde{O}(\epsilon^{-1} + (1-\alpha)^3\alpha^{-3}/\epsilon) = \tilde{O}(\alpha^{-3}\epsilon^{-1}). \end{aligned} \quad (3.56)$$

(b) Finally we sketch the proof that  $\Psi$  is well approximated by an MPS of small bond dimension. We first express it exactly as an MPS of possibly exponential (in  $n$ ) bond dimension and then truncate the MPS cut by cut. It is shown in [146] the error accumulates at most additively: If an inverse polynomial overall error  $1/p(n) = 1/\text{poly}(n)$  is allowed, it suffices that the error of truncating each cut is  $1/(np(n)) = 1/\text{poly}(n)$ . We require that

$$1/\text{poly}(n) = p_i \Rightarrow i = O(\log n), \quad (3.57)$$

and hence the bond dimension is  $2^{\tilde{O}(\epsilon^{-1/4} \log^{3/4} n)}$ .  $\square$

### 3.5 Notes

For non-degenerate systems ( $f = 1$ ), the upper bound claimed in [10] on the von Neumann entanglement entropy is  $\tilde{O}(\epsilon^{-1})$ . However, the proof in [10] of this claim appears incomplete. Specifically, in Lemma 6.3 in [10]  $t_0$  should be at least  $O(\epsilon_0/\epsilon^2 + \epsilon^{-1})$  in order that the robustness theorem (Theorem 6.1 in [10]) applies to  $H^{(t_0)}$ , i.e., the robustness theorem does not guarantee that  $H^{(t_0)}$  is gapped if  $t_0 = O(1)$ . Then  $s = \tilde{O}(\epsilon^{-1})$  (and  $l = s^2$ ) does not give an AGSP for  $H^{(t_0)}$  with  $\Delta D \leq 1/2$ , but  $s = \tilde{O}(\epsilon^{-3/2})$  does. A straightforward calculation shows that the upper bound  $\tilde{O}(\epsilon^{-3/2})$  on the von Neumann entanglement entropy follows from the proof in [10]. Nevertheless, in this chapter we have shown that the claim in [10] is correct, because Theorem 2 (as a stronger version of the robustness theorem) only requires  $t \geq O(\log \epsilon^{-1})$ .

After the appearance of this chapter on arXiv [70], Section 3.2 (perturbation theory) was extended to higher dimensions [11]. In particular, Theorems 4.2, 4.6 in [11] are generalizations of Lemmas 3, 4, respectively.

# Chapter 4

## Efficient algorithm for ground states in gapped spin chains

A (deterministic) polynomial-time algorithm is proposed for approximating the ground state of (general) 1D gapped Hamiltonians. Let  $\epsilon, n, \eta$  be the energy gap, the system size, and the desired precision, respectively. Neglecting  $\epsilon$ -dependent sub-polynomial (in  $n$ ) and constant factors, the running time of the algorithm is  $n^{O(1/\epsilon)}$  for  $\eta = n^{-O(1)}$  and is  $n^{O(1)}$  for  $\eta = n^{-o(1)}$ .

### 4.1 Introduction and background

Computing the ground state in quantum many-body systems with local interactions is a fundamental problem in condensed matter physics. Intuitively, this problem is likely intractable because the dimension of the Hilbert space of the system grows exponentially with the system size. Indeed, computing the ground-state energy of 1D Hamiltonians is QMA-complete [7, 58]. Therefore, (assuming QMA $\neq$ NP) ground states of 1D Hamiltonians do not in general have classical representations from which physical properties can be efficiently extracted. It should be emphasized that the local Hamiltonians constructed in all known proofs of the QMA-hardness are gapless. Indeed, the ground state of 1D gapped Hamiltonians can be [59, 10, 70] efficiently represented as an MPS [118, 41], a data structure that allows efficient computation of physical observables. Thus, the 1D gapped local Hamiltonian problem is in NP.

In practice, the DMRG algorithm [161, 162] is highly successful in 1D gapped systems, and moderately successful in a large class of 1D gapless systems. It is the leading numerical method in 1D and is now running on the computers of condensed matter physicists everywhere on earth. Despite its remarkable popularity, DMRG is still a heuristic local search algorithm over MPS: It can get stuck in a local minimum and there is no guarantee that it always converges in polynomial time. The worst-case performance of DMRG-like algorithms has been a long-standing problem for more than two decades. Is there a variant of DMRG that provably finds the ground state of 1D gapped Hamiltonians in polynomial time, or is

the 1D gapped local Hamiltonian problem in P? We are in a situation reminiscent of the practical success of the simplex algorithm for linear programming before the advent of the ellipsoid and interior-point methods.

A lot of progress has been made. Without assuming an energy gap, the ground-state energy of 1D commuting Hamiltonians can be computed efficiently using dynamic programming [135, 5]. This algorithm also provably finds the ground state of 1D gapped Hamiltonians in sub-exponential time [10]. Recently, Landau, Vazirani, and Vidick [95] proposed a randomized polynomial-time algorithm for approximating the ground state of “almost frustration-free” 1D gapped Hamiltonians (see the remark on Lemma 12 for an explanation of this result). However, settling the complexity of the 1D gapped local Hamiltonian problem is still highly desirable because (a) a generic Hamiltonian is not almost frustration-free; (b) frustration-free Hamiltonians are expected to be easier to solve, e.g., they do not suffer from the so-called sign problem in quantum Monte Carlo simulations.

In this chapter, a (deterministic) polynomial-time algorithm is proposed for approximating the ground state of (general) 1D gapped Hamiltonians, i.e., we prove that the 1D gapped local Hamiltonian problem is in P. This algorithm not only has a broader scope, but is also significantly faster than the algorithm in [95]. As an immediate corollary, adiabatic quantum computation with a final 1D gapped Hamiltonian can be efficiently simulated classically and (assuming  $\text{BQP} \neq \text{P}$ ) is therefore not universal, improving Hastings’ result [61] that adiabatic quantum computation with a path of 1D gapped Hamiltonians allows efficient classical simulation.

## 4.2 Main results

Suppose we are working with a chain of  $n$  spins (qudits), and the local dimension  $d = \Theta(1)$  of each spin is an absolute constant. Let  $\mathcal{H}_i = \mathbf{C}^d$  be the Hilbert space of the spin  $i$ ; define  $\mathcal{H}_{[i,j]} = \bigotimes_{k=i}^j \mathcal{H}_k$  as the Hilbert space of the spins with indices in the interval  $[i, j]$  and  $\mathcal{H} = \mathcal{H}_{[1,n]}$  as the Hilbert space of the system. Since the standard bra-ket notation can be cumbersome, in most but not all cases quantum states and their inner products are simply denoted by  $\psi, \phi \dots$  and  $\langle \psi, \phi \rangle$ , respectively, cf.  $\| |\psi\rangle - |\phi\rangle \|$  versus  $\| \psi - \phi \|$ . All states are normalized unless otherwise stated.

Let  $H = \sum_{i=1}^{n-1} H_i$  be a 1D Hamiltonian, where  $H_i$  acts on the spins  $i$  and  $i + 1$  (nearest-neighbor interaction). Assume without loss of generality that the ground-state energy of each  $H_i$  is zero, and  $H_i \leq 1$ . Let  $\epsilon_0$  denote the ground-state energy of  $H$ , which is a measure of how frustrated  $H$  is:  $H$  is frustration-free if  $\epsilon_0 = 0$ , and  $H$  is “almost frustration-free” if  $\epsilon_0 = O(1)$ . Suppose  $H$  has a unique ground state  $\Psi_0$ , and there is a constant gap  $\epsilon$  between the energies of the ground state and the first excited state. It is easy to see  $\epsilon \leq 1$ . The goal is to find an efficient MPS approximation to the ground state of  $H$ .

**Definition 5** (MPS [118, 41]). Let  $\{|j_i\rangle\}_{j_i=1}^d$  be the computational basis of  $\mathcal{H}_i$  and  $\{D_i\}_{i=0}^n$

with  $D_0 = D_n = 1$  be a sequence of positive integers. An MPS  $\Psi$  takes the form

$$\Psi = \sum_{j_1, j_2, \dots, j_n=1}^d A_{j_1}^{[1]} A_{j_2}^{[2]} \cdots A_{j_n}^{[n]} |j_1 j_2 \cdots j_n\rangle, \quad (4.1)$$

where  $A_{j_i}^{[i]}$  is a matrix of size  $D_{i-1} \times D_i$ . Define  $D = \max\{D_i\}_{i=0}^n$  as the bond dimension of the MPS  $\Psi$ .

Clearly, an MPS representation is efficient if its bond dimension is (at most) a polynomial in  $n$ . The existence of an efficient MPS approximation to the ground state of 1D gapped Hamiltonians is a by-product of the proof of the area law for entanglement [59, 10, 70]. Let  $\tilde{O}(x) := O(x \text{ polylog } x)$  hide a polylogarithmic factor, and suppose the desired precision  $\eta = n^{-O(1)}$  is lower bounded by an inverse polynomial in  $n$ .

**Lemma 10** ([10, 70]). *There exists an MPS  $\Psi$  of bond dimension  $D = 2^{\tilde{O}(1/\epsilon + \epsilon^{-1/4} \log^{3/4}(n/\eta))}$  such that  $|\langle \Psi, \Psi_0 \rangle| \geq 1 - \eta$ .*

As a corollary, the ground state of 1D gapped Hamiltonians can be computed in sub-exponential time using dynamic programming.

**Lemma 11** ([10, 135, 5]). *In 1D gapped systems there is a  $2^{2^{\tilde{O}(\epsilon^{-1/4} \log^{3/4} n)}}$ -time algorithm that outputs an MPS  $\Psi$  such that  $|\langle \Psi, \Psi_0 \rangle| \geq 1 - \eta$ .*

Recently, Landau, Vazirani, and Vidick [95] proposed a randomized polynomial-time algorithm for approximating the ground state of almost frustration-free 1D gapped Hamiltonians.

**Lemma 12** ([95]). *In almost frustration-free 1D gapped systems there is a randomized polynomial-time algorithm that outputs an MPS  $\Psi$  such that  $|\langle \Psi, \Psi_0 \rangle| \geq 1 - \eta$  with probability at least  $1 - 1/\text{poly } n$ . Its running time is  $n^{2^{\tilde{O}(1/\epsilon)}}$  for  $\eta = n^{-O(1)}$  and is still  $n^{2^{\tilde{O}(1/\epsilon)}}$  for  $\eta = n^{-o(1)}$ .*

*Remark.* In general 1D gapped systems the running time of this algorithm is  $n^{2^{\tilde{O}(1/\epsilon)} + O(\epsilon_0/\epsilon)}$  and may be exponential in  $n$  if  $\epsilon_0 = \Theta(n)$ . In frustration-free 1D gapped systems this algorithm can be derandomized using the detectability lemma [6]. See Section 4.7 for details.

Some  $\epsilon$ -dependent sub-polynomial (e.g.,  $2^{\tilde{O}(\epsilon^{-1/4} \log^{3/4} n)}$ ) and constant (e.g.,  $2^{2^{\tilde{O}(1/\epsilon)}}$ ) factors will appear below. If not dominant (e.g., accompanied with  $\text{poly } n$ ), depending on the context they may be neglected or kept for simplicity or clarity, respectively. The main result of this chapter is

**Theorem 3.** *In (general) 1D gapped systems there is a (deterministic) polynomial-time algorithm that outputs an MPS  $\Psi$  such that  $\langle \Psi, H\Psi \rangle \leq \epsilon_0 + \eta\epsilon$ . Its running time is  $n^{O(1/\epsilon)}$  for  $\eta = n^{-O(1)}$  and is  $n^{O(1)}$  for  $\eta = n^{-o(1)}$ .*

*Remark.* It is easy to see that  $\langle \Psi, H\Psi \rangle \leq \epsilon_0 + \eta\epsilon$  implies  $|\langle \Psi, \Psi_0 \rangle| \geq 1 - \eta$ .

Hastings [61] proved that adiabatic quantum computation with a path of 1D gapped Hamiltonians allows efficient classical simulation and (assuming  $\text{BQP} \neq \text{P}$ ) is therefore not universal. Suppose  $H(t)$  with  $0 \leq t \leq t_{max} \leq \text{poly } n$  is a “smooth” path of 1D Hamiltonians, where the ground state of  $H(0)$  is a simple product state. Let  $\Psi_0(t)$  and  $\epsilon(t)$  be the ground state and the energy gap of  $H(t)$ , respectively.

**Lemma 13** ([61]). *Suppose  $H(t)$  has a constant energy gap for  $0 \leq t \leq t_{max}$ . Then there is a polynomial-time algorithm that outputs an MPS  $\Psi$  such that  $|\langle \Psi, \Psi_0(t_{max}) \rangle| \geq 1 - \eta$ . Its running time is  $n^{O(1/\min_{0 \leq t \leq t_{max}} \{\epsilon(t)\})}$  for  $\eta = n^{-O(1)}$  and is still  $n^{O(1/\min_{0 \leq t \leq t_{max}} \{\epsilon(t)\})}$  for  $\eta = n^{-o(1)}$ .*

As an immediate corollary of Theorem 3, adiabatic quantum computation with a final 1D gapped Hamiltonian can be efficiently simulated classically. Suppose  $H(t_{max})$  has a constant energy gap. Then our algorithm outputs an MPS  $\Psi$  such that  $|\langle \Psi, \Psi_0(t_{max}) \rangle| \geq 1 - \eta$ . Its running time is  $n^{O(1/\epsilon(t_{max}))}$  for  $\eta = n^{-O(1)}$  and is  $n^{O(1)}$  for  $\eta = n^{-o(1)}$ .

### 4.3 Overview

The outline of our algorithm is similar to that in Lemma 12. We begin by defining the notion of “support set” (known as “viable set” in [95]).

**Definition 6** (support set).  $S \subseteq \mathcal{H}_{[1,i]}$  is an  $(i, s, b, \delta \text{ or } \Delta)$ -support set if there exists a state  $\psi \in \mathcal{H}$  (called a witness for  $S$ ) such that

- (i) the reduced density matrix of  $\psi$  on  $\mathcal{H}_{[1,i]}$  is supported on  $\text{span } S$ ;
- (ii)  $|S| \leq s$ ;
- (iii) all elements in  $S$  are MPS of bond dimension at most  $b$ ;
- (iv)  $|\langle \psi, \Psi_0 \rangle| \geq 1 - \delta$  or  $\langle \psi, H\psi \rangle \leq \epsilon_0 + \Delta\epsilon$  (depending on the context either  $\delta$  or  $\Delta$  is used as the precision parameter).

*Remark.* Lemma 14 implies that an  $(i, s, b, \Delta = \eta)$ -support set is also an  $(i, s, b, \delta = \eta)$ -support set.

Our algorithm iteratively constructs an  $(i, p_1 p_3, p_2 p_3, \Delta = c\epsilon^6)$ -support set  $S_i$  for  $i = 1, 2, \dots, n-1$ , where  $p_1, p_2, p_3$  are (upper bounded by)  $i$ -independent and  $\epsilon$ -dependent polynomials in  $n$ , and  $c$  is a sufficiently small absolute constant. The  $n$ th iteration is slightly different and constructs an  $(n, p_1 p_4, p_2 p_4, \Delta = \eta)$ -support set  $S_n$ , where  $p_4$  is again a polynomial in  $n$ . After the last iteration, we obtain an MPS approximation to the ground state  $\Psi_0$  of  $H$  from the last support set  $S_n$  by minimizing the energy over the subspace  $\text{span } S_n$ . The solution has the desired precision  $\eta$ , and the minimization can be formulated as a convex program of polynomial size. Indeed,  $\text{span } S_n$  is of polynomial dimension, and any element in  $\text{span } S_n$  is an MPS of polynomial bond dimension.

Table 4.1: Evolution of the parameters in each iteration. The asterisks mark the parameter that is reduced at every step.

	$i$	$s$	$b$	$\delta$	$\Delta$
start	$i - 1$	$p_1 p_3$	$p_2 p_3$	n/a	$c\epsilon^6$
<b>extension</b>	$i$	$d p_1 p_3$	$p_2 p_3$	n/a	$c\epsilon^6$
<b>cardinality reduction</b>	$i$	$p_1^*$	$d p_1 p_2 p_3^2$	1/1000	1/1000
<b>bond truncation</b>	$i$	$p_1$	$p_2^*$	1/20	n/a
<b>error reduction</b> ( $i \leq n - 1$ )	$i$	$p_1 p_3$	$p_2 p_3$	n/a	$c\epsilon^{6*}$
<b>error reduction</b> ( $i = n$ )	$n$	$p_1 p_4$	$p_2 p_4$	$\eta^*$	$\eta^*$

Each iteration consists of four steps: **extension**, **cardinality reduction**, **bond truncation**, and **error reduction**. Table 4.1 summarizes the evolution of the parameters  $s, b, \delta$  or  $\Delta$  in each iteration of our algorithm.

We briefly recall the algorithm in Lemma 12. This algorithm only uses  $\delta$  as the precision parameter, which is reduced to  $O(\epsilon^2/n)$  at the end of the  $i$ th iteration for  $i = 1, 2, \dots, n - 1$ . The analysis in [95] gives

$$p_1 = n^{2^{\tilde{O}(1/\epsilon)}}, p_2 = n^{2^{\tilde{O}(\epsilon^{-1/4} \log^{3/4} n)}}, p_3 = n^{O(1/\epsilon)}, p_4 = n^{O(1/\epsilon)} \quad (4.2)$$

in almost frustration-free 1D gapped systems. The running time of the algorithm is a polynomial in  $p_1, p_2, p_3, p_4$ , and is dominated by  $p_1$ . Specifically, **extension** is trivial; the analysis of **cardinality reduction** determines  $p_1$ ; **bond truncation** is straightforward; **error reduction** is the only step that involves randomness (it succeeds with probability at least  $1 - 1/\text{poly } n$ ) and the only step that requires  $\epsilon_0 = O(1)$ . Indeed,  $p_3 = n^{O(1/\epsilon + \epsilon_0/\epsilon)}$  and  $p_4 = n^{O(1/\epsilon + \epsilon_0/\epsilon)}$  in general 1D gapped systems. See Section 4.7 for details.

In this chapter, we significantly improve the analysis of **cardinality reduction** using perturbation theory (the truncation lemma [10, 70]) so that  $p_1 = 2^{2^{\tilde{O}(1/\epsilon)}}$  no longer dominates the running time of the algorithm. More importantly, we redesign **error reduction** so that  $p_3 = n^{O(1)}$  and  $p_4 = n^{O(1 + \sqrt{\log(1/\eta)/\log n/\epsilon})}$  in general 1D gapped systems (clearly,  $p_4 = n^{O(1/\epsilon)}$  for  $\eta = n^{-O(1)}$  and  $p_4 = n^{O(1)}$  for  $\eta = n^{-o(1)}$ ). This is achieved using the Fourier transform and the Lieb-Robinson bound [100] but not randomness. **Extension** and **bond truncation** remain unchanged.

## 4.4 Preliminaries

**Lemma 14.**  $\langle \psi, H\psi \rangle \leq \epsilon_0 + \eta\epsilon$  implies  $|\langle \psi, \Psi_0 \rangle| \geq |\langle \psi, \Psi_0 \rangle|^2 \geq 1 - \eta$ .

*Proof.* The state  $\psi$  can be decomposed as  $\psi = c_0\Psi_0 + c_1\Psi_1$ , where  $\Psi_1 \perp \Psi_0$  and  $\langle \Psi_1, H\Psi_1 \rangle \geq \epsilon_0 + \epsilon$ .

$$\epsilon_0 + \eta\epsilon \geq \langle \psi, H\psi \rangle \geq |c_0|^2\epsilon_0 + |c_1|^2(\epsilon_0 + \epsilon) = \epsilon_0 + |c_1|^2\epsilon \Rightarrow |c_0|^2 = 1 - |c_1|^2 \geq 1 - \eta. \quad (4.3)$$

□

**Lemma 15.**  $|\langle \psi, \phi_1 \rangle| \geq 1 - \eta_1$  and  $|\langle \psi, \phi_2 \rangle| \geq 1 - \eta_2$  imply  $|\langle \phi_1, \phi_2 \rangle| \geq 1 - 2(\eta_1 + \eta_2)$ .

*Proof.* Let  $\theta_1$  be the angle between  $\psi$  and  $\phi_1$ , and  $\theta_2$  be the angle between  $\psi$  and  $\phi_2$ .

$$\begin{aligned} |\langle \phi_1, \phi_2 \rangle| &\geq \cos(\theta_1 + \theta_2) = \cos \theta_1 \cos \theta_2 - \sqrt{(1 - \cos^2 \theta_1)(1 - \cos^2 \theta_2)} \\ &\geq (1 - \eta_1)(1 - \eta_2) - \sqrt{(2\eta_1 - \eta_1^2)(2\eta_2 - \eta_2^2)} \geq 1 - 2(\eta_1 + \eta_2). \end{aligned} \quad (4.4)$$

□

**Lemma 16.**  $|\langle \psi, \phi \rangle| \geq 1 - \eta$  implies  $|\langle \psi, \hat{O}\psi \rangle - \langle \phi, \hat{O}\phi \rangle| \leq 2\sqrt{2\eta}$  for any operator  $\hat{O}$  with  $\|\hat{O}\| \leq 1$ .

*Proof.* Assume without loss of generality that  $\langle \psi, \phi \rangle$  is a positive real number.

$$\begin{aligned} \|\psi - \phi\|^2 &= 2 - 2\langle \psi, \phi \rangle \leq 2\eta \text{ and } \langle \psi, \hat{O}\psi \rangle - \langle \phi, \hat{O}\phi \rangle = \langle \psi - \phi, \hat{O}\psi \rangle + \langle \phi, \hat{O}(\psi - \phi) \rangle \\ \Rightarrow |\langle \psi, \hat{O}\psi \rangle - \langle \phi, \hat{O}\phi \rangle| &\leq \|\psi - \phi\| \cdot \|\hat{O}\| \cdot \|\psi\| + \|\phi\| \cdot \|\hat{O}\| \cdot \|\psi - \phi\| \leq 2\sqrt{2\eta}. \end{aligned} \quad (4.5)$$

□

**Definition 7** (truncation). Let  $\psi = \sum_{j \geq 1} \lambda_j l_j \otimes r_j$  be the Schmidt decomposition of a state  $\psi \in \mathcal{H}$  across the cut  $i|i+1$ , where the Schmidt coefficients are in descending order:  $\lambda_1 \geq \lambda_2 \geq \dots > 0$ . Define  $\text{trunc}_D \psi = \sum_{j=1}^D \lambda_j l_j \otimes r_j$ .

**Lemma 17** (Eckart-Young theorem [39]). *The state  $\psi' = \text{trunc}_D \psi / \|\text{trunc}_D \psi\|$  satisfies  $\langle \psi', \psi \rangle \geq |\langle \phi, \psi \rangle|$  for any state  $\phi \in \mathcal{H}$  of Schmidt rank  $D$  (across the cut  $i|i+1$ ).*

**Lemma 18** ([95]). *Suppose  $\phi \in \mathcal{H}$  is a state of Schmidt rank  $D$  (across the cut  $i|i+1$ ).*

$$|\langle \text{trunc}_{D/\eta} \psi, \phi \rangle| \geq |\langle \psi, \phi \rangle| - \eta, \quad \forall \eta > 0, \psi \in \mathcal{H}. \quad (4.6)$$

*Remark.* This is a simple corollary of Lemma 17.

**Lemma 19.**  $\langle \Psi'_0, \Psi_0 \rangle \geq 1 - \eta$  for  $\Psi'_0 = \text{trunc}_{B_\eta} \Psi_0 / \|\text{trunc}_{B_\eta} \Psi_0\|$ , where  $B_\eta = 2^{\tilde{O}(1/\epsilon + \epsilon^{-1/4} \log^{3/4}(1/\eta))}$ .

*Proof.* As a by-product of the proof of the area law for entanglement [70], there exists a state  $\phi \in \mathcal{H}$  of Schmidt rank  $B_\eta$  such that  $\langle \phi, \Psi_0 \rangle \geq 1 - \eta$ . Then, this lemma follows from Lemma 17. □

**Lemma 20.**  $\epsilon \leq 1$ .

*Proof.* It suffices to find two orthogonal states with energies at most  $\epsilon_0 + 1$ . Let  $\{|j_1\rangle\}_{j_1=1}^d$  be the computational basis of  $\mathcal{H}_1$ , and  $\psi \in \mathcal{H}_{[2,n]}$  be the ground state of  $\sum_{i=2}^{n-1} H_i$ . For any  $|j_1\rangle$ ,

$$\langle j_1 \psi, H j_1 \psi \rangle = \langle j_1 \psi, H_1 j_1 \psi \rangle + \left\langle \psi, \sum_{i=2}^{n-1} H_i \psi \right\rangle \leq \langle \Psi_0, H_1 \Psi_0 \rangle + 1 + \left\langle \Psi_0, \sum_{i=2}^{n-1} H_i \Psi_0 \right\rangle = \epsilon_0 + 1. \quad (4.7)$$

□



**Lemma 21.**  $\langle \psi, H\psi \rangle \leq \epsilon_0 + \eta\epsilon$  and  $\eta \leq 1/10$  imply  $\langle \psi', H\psi' \rangle \leq \epsilon_0 + 25\sqrt{\eta}$  for  $\psi' = \text{trunc}_{B_\eta} \psi / \|\text{trunc}_{B_\eta} \psi\|$ .

*Proof.* Lemma 14 implies  $|\langle \psi, \Psi_0 \rangle| \geq 1 - \eta$ . Since  $|\langle \Psi'_0, \Psi_0 \rangle| \geq 1 - \eta$  for  $\Psi'_0 = \text{trunc}_{B_\eta} \Psi_0 / \|\text{trunc}_{B_\eta} \Psi_0\|$  (Lemma 19), Lemma 15 implies  $|\langle \psi, \Psi'_0 \rangle| \geq 1 - 4\eta$ . Let  $\phi' = \text{trunc}_{B_\eta} \psi$  and  $\psi = \phi' + \phi$ . Lemma 17 implies  $\|\phi'\| = \langle \psi, \phi' \rangle / \|\phi'\| \geq 1 - 4\eta$ . Hence,  $\|\phi\|^2 = 1 - \|\phi'\|^2 \leq 8\eta$ . Since  $\eta \leq 1/10$ ,

$$\begin{aligned} \langle \psi, (H - H_i)\psi \rangle &= \langle \phi', (H - H_i)\phi' \rangle + \langle \phi, (H - H_i)\phi \rangle \\ &\Rightarrow \langle \phi', H\phi' \rangle = \langle \psi, H\psi \rangle - \langle \phi, H\phi \rangle + \langle \phi, H_i\phi \rangle - \langle \phi', H_i\phi \rangle - \langle \phi, H_i\psi \rangle \\ &\leq \epsilon_0 + \eta\epsilon - \epsilon_0\|\phi\|^2 + \|\phi\|^2 + 2\|\phi\| \leq \epsilon_0\|\phi'\|^2 + \eta\epsilon + 8\eta + 4\sqrt{2\eta} \\ &\Rightarrow \langle \psi', H\psi' \rangle \leq \epsilon_0 + (\eta\epsilon + 8\eta + 4\sqrt{2\eta})/(1 - 4\eta)^2 \leq \epsilon_0 + 25\sqrt{\eta}. \end{aligned} \quad (4.8)$$

□

**Definition 8** (matrix product operator (MPO)). Let  $\{\hat{O}_{j_i}\}_{j_i=1}^{d^2}$  be a basis of the space of operators on  $\mathcal{H}_i$  and  $\{D_i\}_{i=0}^n$  with  $D_0 = D_n = 1$  be a sequence of positive integers. As the operator analog of MPS, an MPO  $K$  takes the form

$$K = \sum_{j_1, j_2, \dots, j_n=1}^{d^2} \left( A_{j_1}^{[1]} A_{j_2}^{[2]} \dots A_{j_n}^{[n]} \right) \hat{O}_{j_1} \otimes \hat{O}_{j_2} \otimes \dots \otimes \hat{O}_{j_n}, \quad (4.9)$$

where  $A_{j_i}^{[i]}$  is a matrix of size  $D_{i-1} \times D_i$ . Define  $D = \max\{D_i\}_{i=0}^n$  as the bond dimension of the MPO  $K$ .

## 4.5 Algorithm and analysis

In the  $i$ th iteration our algorithm constructs an  $(i, p_1 p_3, p_2 p_3, \Delta = c\epsilon^6)$ -support set  $S_i$  from an  $(i-1, p_1 p_3, p_2 p_3, \Delta = c\epsilon^6)$ -support set  $S_{i-1}$  returned in the  $(i-1)$ th iteration.

### Extension

**Extension** is trivial. Let  $\{|j_i\rangle\}_{j_i=1}^d$  be the computational basis of  $\mathcal{H}_i$ . It is easy to see that  $S_i^{(1)} := \{\psi|j_i\rangle : \forall \psi \in S_{i-1}, j_i = 1, 2, \dots, d\}$  is an  $(i, dp_1 p_3, p_2 p_3, \Delta = c\epsilon^6)$ -support set.

### Cardinality reduction

Dynamic programming for MPS is the essential ingredient of **cardinality reduction**. It was first developed by [135, 5] and then reformulated using the notion of “boundary contraction” [95].

### Boundary contraction

Let  $\text{tr}_{[i,j]} \rho$  denote the partial trace over  $\mathcal{H}_{[i,j]}$  of a density matrix  $\rho$  on  $\mathcal{H}$ .

**Definition 9** (boundary contraction). Let  $\psi = \sum_{j=1}^B \lambda_j l_j \otimes r_j$  be the Schmidt decomposition of a state  $\psi \in \mathcal{H}$  across the cut  $i|i+1$ . Let  $\{|j\rangle\}_{j=1}^B$  be the computational basis of  $\mathbf{C}^B$ . Let  $U_\psi : \mathbf{C}^B \rightarrow \mathcal{H}_{[i+1,n]}$  be the isometry specified by  $U_\psi |j\rangle = r_j$  such that  $U_\psi^{-1} \psi = \sum_{j=1}^B \lambda_j l_j |j\rangle \in \mathcal{H}_{[1,i]} \otimes \mathbf{C}^B$ . The boundary contraction  $\text{cont } \psi$  is a density matrix on  $\mathcal{H}_i \otimes \mathbf{C}^B$ :

$$\text{cont } \psi := U_\psi^{-1} \text{tr}_{[1,i-1]}(|\psi\rangle\langle\psi|) U_\psi. \quad (4.10)$$

Let  $\epsilon_L, \epsilon_R$  be the ground-state energies of  $H_L := \sum_{j=1}^{i-1} H_j$  and  $H_R := \sum_{j=i+1}^{n-1} H_j$ , respectively. Define  $H'_L = H_L - \epsilon_L$  and  $H'_R = H_R - \epsilon_R$  so that the ground-state energies of  $H'_L, H'_R$  are 0.

**Lemma 22.** *Let  $\rho$  be a density matrix on  $\mathcal{H}_{[1,i]} \otimes \mathbf{C}^B$  and  $\psi = \sum_{j=1}^B \lambda_j l_j \otimes r_j$  be the Schmidt decomposition of a state  $\psi \in \mathcal{H}$  (across the cut  $i|i+1$ ). The density matrix  $\rho' := U_\psi \rho U_\psi^{-1}$  on  $\mathcal{H}$  has energy*

$$\text{tr}(\rho' H) \leq \text{tr}(\rho H_L) + \langle \psi, (H_i + H_R) \psi \rangle + \|\text{tr}_{[1,i-1]} \rho - \text{cont } \psi\|_1 \left( 1 + \max_{r \in \text{span}\{r_j\}} \|H'_R r\| \right). \quad (4.11)$$

*Proof.* Since  $U_\psi$  is an isometry,

$$\begin{aligned} & \text{tr}(\rho' H) - \text{tr}(\rho H_L) - \langle \psi, (H_i + H_R) \psi \rangle = \text{tr}(\rho' H) - \text{tr}(\rho' H_L) - \langle \psi, (H_i + H_R) \psi \rangle \\ & = \text{tr}(\rho' (H_i + H_R)) - \langle \psi, (H_i + H_R) \psi \rangle = \text{tr}[(\rho' - |\psi\rangle\langle\psi|)(H_i + H_R)] \\ & = \text{tr}[(\rho' - |\psi\rangle\langle\psi|)(H_i + H'_R)] = \text{tr}[\text{tr}_{[1,i-1]}(\rho' - |\psi\rangle\langle\psi|)(H_i + H'_R)] \\ & = \text{tr}[U_\psi^{-1} \text{tr}_{[1,i-1]}(\rho' - |\psi\rangle\langle\psi|) U_\psi U_\psi^{-1} (H_i + H'_R) U_\psi] \\ & = \text{tr}[(\text{tr}_{[1,i-1]} \rho - \text{cont } \psi)(U_\psi^{-1} H_i U_\psi + U_\psi^{-1} H'_R U_\psi)] \\ & \leq \|\text{tr}_{[1,i-1]} \rho - \text{cont } \psi\|_1 \cdot \|U_\psi^{-1} H_i U_\psi + U_\psi^{-1} H'_R U_\psi\| \\ & \leq \|\text{tr}_{[1,i-1]} \rho - \text{cont } \psi\|_1 (1 + \|U_\psi^{-1} H'_R U_\psi\|) \\ & \leq \|\text{tr}_{[1,i-1]} \rho - \text{cont } \psi\|_1 \left( 1 + \max_{r \in \text{span}\{r_j\}} \|H'_R r\| \right). \end{aligned} \quad (4.12)$$

□

### Algorithm

Let  $N$  be a  $\xi$ -net with  $\xi = \tilde{\Omega}(\epsilon)$  for the trace norm over the space of boundary contractions of bond dimension  $B_{8\sqrt{c}\epsilon^2} = 2^{\tilde{O}(1/\epsilon)}$  so that  $|N| = (B/\xi)^{O(B)} = 2^{2^{\tilde{O}(1/\epsilon)}}$ . It is straightforward to construct  $N$  in time  $\text{poly } |N| = 2^{2^{\tilde{O}(1/\epsilon)}}$ .

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**Cardinality reduction convex program and bond truncation**

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0. Let the variable  $\rho$  be a density matrix on  $\text{span } S_i^{(1)} \otimes \mathbf{C}^{B_{8\sqrt{c}\epsilon^2}} \subseteq \mathcal{H}_{[1,i]} \otimes \mathbf{C}^{B_{8\sqrt{c}\epsilon^2}}$ .  
 1. For each  $X \in N$ , solve the convex program:

$$\min \text{tr}(\rho H_L); \text{ s. t. } \|\text{tr}_{[1,i-1]} \rho - X\|_1 \leq \xi, \quad \text{tr} \rho = 1, \quad \rho \geq 0. \quad (4.13)$$

2. Let  $\varphi = \sum_j \varphi_j |j\rangle$  be the eigenvector of the solution  $\rho$  with the largest eigenvalue.  
 3. Let  $\varphi' = \sum_j \varphi'_j |j\rangle$  be the state obtained by truncating each bond (in whatever order) of  $\varphi$  to  $p_2$ .  
 4.  $S_i^{(3)}$  consists of the MPS representations of all  $\varphi'_j$ .
- 

**Analysis**

Let  $P_t$  be the projection onto the subspace  $\mathcal{H}_R^{\leq t}$  spanned by the eigenvectors of  $H'_R$  with eigenvalues at most  $t$ , and  $Q_t$  be the projection onto the subspace spanned by the eigenvectors of  $H'_L + H'_R$  with eigenvalues at most  $t$ .

**Lemma 23** (truncation lemma).

$$\|(1 - P_t)\Psi_0\| \leq \|(1 - Q_t)\Psi_0\| \leq 100 \cdot 2^{-t/20}. \quad (4.14)$$

*Proof.* The first inequality is obvious:  $P_t \geq Q_t$  as  $[H'_L, H'_R] = 0$  and  $H'_L \geq 0$ . The second inequality was proved in [10].  $\square$

Let  $t = O(\log(1/\epsilon))$  so that  $100 \cdot 2^{-t/20} \leq c\epsilon^6$ .

**Lemma 24.** *There exists a state  $\psi \in \text{span } S_i^{(1)} \otimes \mathcal{H}_R^{\leq t}$  of Schmidt rank  $B_{8\sqrt{c}\epsilon^2}$  (across the cut  $i|i+1$ ) such that  $\langle \psi, H\psi \rangle \leq \epsilon_0 + 200c^{1/4}\epsilon$ .*

*Proof.* Let  $\phi$  be a witness for  $S_i^{(1)}$ . Since  $S_i^{(1)}$  is an  $(i, dp_1p_3, p_2p_3, \Delta = c\epsilon^6)$ -support set, Lemma 14 implies  $|\langle \phi, \Psi_0 \rangle| \geq 1 - c\epsilon^6$ . Lemma 16 implies  $\langle \phi, H_i\phi \rangle \geq \langle \Psi_0, H_i\Psi_0 \rangle - 2\sqrt{2}c\epsilon^3$ . Let  $\phi' = P_t\phi/\|P_t\phi\|$  so that  $\phi' \in \text{span } S_i^{(1)} \otimes \mathcal{H}_R^{\leq t}$  by construction. Since the state  $\phi$  has energy at most  $\epsilon_0 + c\epsilon^7$ ,

$$\begin{aligned} \langle \Psi_0, (H'_L + H'_R)\Psi_0 \rangle + 4\sqrt{c}\epsilon^3 &\geq \langle \Psi_0, (H'_L + H'_R)\Psi_0 \rangle + 2\sqrt{2}c\epsilon^3 + c\epsilon^7 \geq \langle \phi, (H'_L + H'_R)\phi \rangle \\ &= \langle \phi, P_t(H'_L + H'_R)P_t\phi \rangle + \langle \phi, (1 - P_t)(H'_L + H'_R)(1 - P_t)\phi \rangle \\ &\geq \langle \phi', (H'_L + H'_R)\phi' \rangle \|P_t\phi\|^2 + t\|(1 - P_t)\phi\|^2. \end{aligned} \quad (4.15)$$

The ground-state energy of  $H'_L + H_i + H'_R$  is at most 1 as  $H_i \leq 1$ . Hence,  $\langle \Psi_0, (H'_L + H'_R)\Psi_0 \rangle \leq 1$  as  $H_i \geq 0$ . (4.15) implies

$$t \gg \langle \Psi_0, (H'_L + H'_R)\Psi_0 \rangle + 4\sqrt{c}\epsilon^3 \Rightarrow \langle \phi', (H'_L + H'_R)\phi' \rangle \leq \langle \Psi_0, (H'_L + H'_R)\Psi_0 \rangle + 4\sqrt{c}\epsilon^3. \quad (4.16)$$

Lemmas 16, 23 imply

$$\begin{aligned}
 |\langle \phi', \Psi_0 \rangle| &\geq |\langle P_t \phi, \Psi_0 \rangle| = |\langle \phi, P_t \Psi_0 \rangle| \geq |\langle \phi, \Psi_0 \rangle| - |\langle \phi, (1 - P_t) \Psi_0 \rangle| \\
 &\geq 1 - c\epsilon^6 - \|(1 - P_t) \Psi_0\| \geq 1 - c\epsilon^6 - 100 \cdot 2^{-t/20} \geq 1 - 2c\epsilon^6 \\
 &\Rightarrow \langle \phi', H_i \phi' \rangle \leq \langle \Psi_0, H_i \Psi_0 \rangle + 4\sqrt{c}\epsilon^3.
 \end{aligned} \tag{4.17}$$

Summing (4.16) (4.17) gives  $\langle \phi', H \phi' \rangle \leq \langle \Psi_0, H \Psi_0 \rangle + 4\sqrt{c}\epsilon^3 + 4\sqrt{c}\epsilon^3 = \epsilon_0 + 8\sqrt{c}\epsilon^3$ . Finally, Lemma 21 implies that the state  $\psi := \text{trunc}_{B_{8\sqrt{c}\epsilon^2}} \phi' / \|\text{trunc}_{B_{8\sqrt{c}\epsilon^2}} \phi'\| \in \text{span } S_i^{(1)} \otimes \mathcal{H}_R^{\leq t}$  has energy  $\langle \psi, H \psi \rangle \leq \epsilon_0 + 75c^{1/4}\epsilon$ .  $\square$

**Lemma 25.**  $S_i^{(2)}$  is an  $(i, p_1, dp_1 p_2 p_3^2, \Delta = 1/1000)$ -support set, where  $S_i^{(2)}$  consists of the MPS representations of all  $\varphi_j$ .

*Proof.* Since  $N$  is a  $\xi$ -net, there is an element  $X \in N$  such that  $\|\text{cont } \psi - X\|_1 \leq \xi$ . Clearly,  $\text{tr}(\rho H_L) \leq \langle \psi, H_L \psi \rangle$  as  $U_\psi^{-1} |\psi\rangle \langle \psi| U_\psi$  is a feasible solution to the convex program (4.13). Let  $\sigma = U_\psi \rho U_\psi^{-1}$ , and set  $\xi = \tilde{\Omega}(\epsilon)$  such that  $2\xi(1+t) \leq \epsilon/4000$ . Lemma 22 implies

$$\begin{aligned}
 \text{tr}(\sigma H) &\leq \text{tr}(\rho H_L) + \langle \psi, (H_i + H_R) \psi \rangle + \|\text{tr}_{[1, i-1]} \rho - \text{cont } \psi\|_1 \left( 1 + \max_{r \in \text{span}\{r_j\}} \|H'_R r\| \right) \\
 &\leq \langle \psi, (H_L + H_i + H_R) \psi \rangle + 2\xi \left( 1 + \max_{r \in \mathcal{H}_R^{\leq t}} \|H'_R r\| \right) \leq \langle \psi, H \psi \rangle + 2\xi(1+t) \\
 &\leq \epsilon_0 + 200c^{1/4}\epsilon + \epsilon/4000 \leq \epsilon_0 + \epsilon/2000
 \end{aligned} \tag{4.18}$$

for sufficiently small constant  $c$ . We observe that

- (1) there exists at least an eigenstate of  $\sigma$  with energy at most  $\epsilon_0 + \epsilon/1000$ ;
- (2) there is at most one such eigenstate as Lemma 14 implies that such an eigenstate is close to  $\Psi_0$ ;
- (3) this eigenstate (denoted by  $\Phi$ ) has the largest eigenvalue due to Markov's inequality in probability theory;
- (4)  $\Phi = U_\psi \varphi$  is a witness for  $S_i^{(2)}$  as an  $(i, p_1, dp_1 p_2 p_3^2, \Delta = 1/1000)$ -support set with  $p_1 = B_{8\sqrt{c}\epsilon^2} |N| = 2^{2\tilde{\delta}(1/\epsilon)}$ .  $\square$

## Bond truncation

The analysis of **bond truncation** follows immediately from Lemmas 10, 18, and is (almost) identical to that in [95].

**Lemma 26.**  $S_i^{(3)}$  is an  $(i, p_1, p_2, \delta = 1/20)$ -support set.

*Proof.* Since  $\Phi$  is a witness for  $S_i^{(2)}$  with energy at most  $\epsilon_0 + \epsilon/1000$ , Lemma 14 implies  $|\langle \Phi, \Psi_0 \rangle| \geq 999/1000$ . Lemma 10 implies the existence of an MPS  $\Psi$  of bond dimension

$2^{\tilde{O}(\epsilon^{-1/4} \log^{3/4} n)}$  such that  $|\langle \Psi, \Psi_0 \rangle| \geq 999/1000$ . Lemma 15 implies  $|\langle \Psi, \Phi \rangle| \geq 249/250$ . Let  $\Phi'$  be the state obtained by truncating each bond to the left of the cut  $i|i+1$  (in the same order as each bond of  $\varphi$  is truncated) of  $\Phi$  to  $p_2 = 1000n2^{\tilde{O}(\epsilon^{-1/4} \log^{3/4} n)}$ . Lemma 18 implies  $|\langle \Psi, \Phi' \rangle| \geq 199/200$ . Lemma 15 implies  $|\langle \Psi_0, \Phi' \rangle| \geq 49/50$ . Hence  $\Phi' = U_\psi \varphi'$  is a witness for  $S_i^{(3)}$  as an  $(i, p_1, p_2, \delta = 1/20)$ -support set.  $\square$

## Error reduction

To reduce the energy of the witness  $\Phi'$ , we efficiently construct an MPO that approximately projects  $\Phi'$  onto the ground state  $\Psi_0$ . This construction was used extensively by Hastings to prove several well-known results (e.g., the 1D area law for entanglement [59]) for the ground state of gapped local Hamiltonians. It applies to general 1D gapped systems and does not involve randomness. It uses the Fourier transform and the Lieb-Robinson bound [100].

Assume for the moment that we have an estimate  $\epsilon'_0$  of the ground-state energy  $\epsilon_0$  of  $H$  in the sense that  $|\epsilon_0 - \epsilon'_0| \leq \epsilon/\sqrt{q} \leq \epsilon/2$ , where  $q = 4 \log(1/\eta) + 24$ . Let

$$A := e^{-\frac{q(H-\epsilon'_0)^2}{2\epsilon^2}} = \frac{\epsilon}{\sqrt{2\pi q}} \int_{-\infty}^{+\infty} e^{-\frac{\epsilon^2 t^2}{2q} - i(H-\epsilon'_0)t} dt. \quad (4.19)$$

**Lemma 27.**  $|\langle \Phi', \Psi_0 \rangle| \geq 19/20$  implies  $\langle \phi, H\phi \rangle \leq \epsilon_0 + \eta\epsilon/100$  for  $\phi = A\Phi'/\|A\Phi'\|$ .

*Proof.* Let  $\{\Psi_j\}_{j=0}^{d^n-1}$  be the eigenvectors of  $H$  with the corresponding eigenvalues  $\{\epsilon_j\}_{j=0}^{d^n-1}$  in ascending order. The state  $\Phi'$  can be decomposed as  $\Phi' = \sum_{j=0}^{d^n-1} c_j \Psi_j$  with  $|c_0| \geq 19/20$ .

$$\|A\Phi'\| \geq |c_0| \cdot \|A\Psi_0\| \geq 19e^{-\frac{q(\epsilon_0-\epsilon'_0)^2}{2\epsilon^2}}/20 \geq 19/(20\sqrt{e}) \geq 1/2. \quad (4.20)$$

Since  $\epsilon_j - \epsilon_0 \leq 2(\epsilon_j - \epsilon'_0)$  for  $j \geq 1$ ,

$$\begin{aligned} \langle \phi, (H - \epsilon_0)\phi \rangle &= \langle A\Phi', (H - \epsilon_0)A\Phi' \rangle / \|A\Phi'\|^2 \leq 4 \sum_{j=1}^{d^n-1} (\epsilon_j - \epsilon_0) |c_j|^2 e^{-q(\epsilon_j - \epsilon'_0)^2/\epsilon^2} \\ &\leq 8 \sum_{j=1}^{d^n-1} (\epsilon_j - \epsilon'_0) |c_j|^2 e^{-\frac{q(\epsilon_j - \epsilon'_0)^2}{\epsilon^2}} \leq 8 \max_{x \geq \epsilon/2} \{x e^{-\frac{qx^2}{\epsilon^2}}\} \sum_{j=1}^{d^n-1} |c_j|^2 \leq 4\epsilon e^{-\frac{q}{4}} \leq \eta\epsilon/100. \end{aligned} \quad (4.21)$$

$\square$

**Lemma 28.** An MPO  $K$  of bond dimension  $D = n^{O(1 + \sqrt{\log(1/\eta)/\log n/\epsilon})}$  can be efficiently constructed such that  $\|K - A\| \leq \eta\epsilon/(1000n) =: \eta'$ .

*Proof.* Following [61], we truncate and discretize the integral in (4.19):

$$\begin{aligned} A &= \frac{\epsilon}{\sqrt{2\pi q}} \int_{-\infty}^{+\infty} e^{-\frac{\epsilon^2 t^2}{2q} - i(H-\epsilon'_0)t} dt \approx \frac{\epsilon}{\sqrt{2\pi q}} \int_{-T}^T e^{-\frac{\epsilon^2 t^2}{2q} - i(H-\epsilon'_0)t} dt \\ &\approx \frac{\epsilon\tau}{\sqrt{2\pi q}} \sum_{j=-T/\tau}^{T/\tau} e^{-\frac{\epsilon^2 \tau^2 j^2}{2q} - i(H-\epsilon'_0)\tau j} \approx \frac{\epsilon\tau}{\sqrt{2\pi q}} \sum_{j=-T/\tau}^{T/\tau} e^{-\frac{\epsilon^2 \tau^2 j^2}{2q}} K_j =: K. \end{aligned} \quad (4.22)$$

The truncation error is of order  $e^{-\epsilon^2 T^2/(2q)} \leq \eta'/3$  for  $T = O(\sqrt{q \log(1/\eta')}/\epsilon)$ . The discretization error is of order  $\epsilon \tau \|H\| T / \sqrt{2\pi q} \leq \eta'/3$  for  $\tau = O(\eta' \sqrt{q}/(\epsilon \|H\| T)) = O(\eta'/(n \sqrt{\log(1/\eta')}))$ . As a consequence of the Lieb-Robinson bound [100], each propagator  $e^{-i(H-\epsilon'_0)\tau j}$  can be approximated to precision  $\eta'/3$  by an MPO  $K_j$  of bond dimension [112]  $2^{O(\tau j)} \text{poly}(n/\eta') = 2^{O(T)} \text{poly}(n/\eta') = 2^{O(\sqrt{q \log(1/\eta')}/\epsilon)} \text{poly}(n/\eta')$ . The number of terms is  $2T/\tau + 1 = O(n \sqrt{q} \log(1/\eta')/(\eta' \epsilon))$ . Therefore, the bond dimension of the MPO  $K$  is  $D = n^{O(1 + \sqrt{\log(1/\eta')/\log n/\epsilon})}$ .  $\square$

Lemmas 27, 28 imply  $\langle \phi', H \phi' \rangle \leq \epsilon_0 + \eta \epsilon / 50$  for  $\phi' = K \Phi' / \|K \Phi'\|$ . Since  $K$  is an MPO of bond dimension  $D$ , it can be decomposed as  $K = \sum_{j=1}^D L_j \otimes R_j$ , where  $L_j$  and  $R_j$  are MPO of bond dimension  $D$  on  $\mathcal{H}_{[1,i]}$  and on  $\mathcal{H}_{[i+1,n]}$ , respectively. It is easy to see that  $S_i := \{L_j \psi : j = 1, 2, \dots, D, \forall \psi \in S_i^{(3)}\}$  is an  $(i, p_1 D, p_2 D, \Delta = \eta)$ -support set. Hence  $p_4 = n^{O(1 + \sqrt{\log(1/\eta)/\log n/\epsilon})}$  for  $i = n$ , and setting  $\eta = c \epsilon^6$  gives  $p_3 = n^{O(1 + \sqrt{\log(1/\epsilon)/\log n/\epsilon})} = n^{O(1)}$  for  $i \leq n - 1$ .

We briefly comment on the assumption that we have an estimate  $\epsilon'_0$  of the ground-state energy  $\epsilon_0$  of  $H$  in the sense that  $|\epsilon_0 - \epsilon'_0| \leq \epsilon/\sqrt{q}$ . Since  $0 \leq \epsilon_0 \leq n$ , we run the whole algorithm with  $\epsilon'_0 = j\epsilon/\sqrt{q}$  and obtain a candidate MPS solution for each  $j = 0, 1, \dots, \lfloor n\sqrt{q}/\epsilon \rfloor$ . The candidate MPS with the lowest energy is identified as the final output.

## 4.6 Degenerate ground states

Previously, we assumed a unique ground state. We now extend the results to 1D gapped systems with degenerate ground states. After the appearance of this chapter on arXiv [69], a different approach of extending results from unique to degenerate ground states was given by [33].

### Main results, overview, and preliminaries

Suppose the ground states of a 1D Hamiltonian  $H = \sum_{i=1}^{n-1} H_i$  are two-fold exactly degenerate (for ease of presentation), and there is a constant energy gap  $\epsilon$ . It should be clear that a minor modification of the proof works for any constant-fold degeneracy and leads to the same results in the presence of an exponentially small  $2^{-\Omega(n)}$  splitting of the degeneracy (as is typically observed in physical systems). The goal is to find efficient MPS approximations to a set of basis vectors of the ground-state space  $G$  of  $H$ . The existence of an efficient MPS approximation to any ground state  $\Psi_0 \in G$  of  $H$  is a by-product of the proof of the area law for entanglement [70].

**Lemma 29** ([70]). *For any ground state  $\Psi_0 \in G$  of  $H$ , there exists an MPS  $\Psi$  of bond dimension  $2^{\tilde{O}(1/\epsilon + \epsilon^{-1/4} \log^{3/4}(n/\eta))}$  such that  $|\langle \Psi, \Psi_0 \rangle| \geq 1 - \eta$ .*

The main result of the present section is

**Theorem 4.** *In 1D gapped systems with two-fold ground-state degeneracy there is a polynomial-time algorithm that outputs two orthogonal MPS  $\Psi, \Psi'$  such that  $\langle \Psi, H\Psi \rangle \leq \epsilon_0 + \eta\epsilon$  and  $\langle \Psi', H\Psi' \rangle \leq \epsilon_0 + \eta\epsilon$ . Its running time is  $n^{O(1/\epsilon)}$  for  $\eta = n^{-O(1)}$  and is  $n^{O(1)}$  for  $\eta = n^{-o(1)}$ .*

*Remark.* Lemma 32 implies that any state in  $\text{span}\{\Psi, \Psi'\}$  has energy at most  $\epsilon_0 + 2\eta\epsilon$ .

**Definition 10** (support set).  $S \subseteq \mathcal{H}_{[1,i]}$  is an  $(i, s, b, \delta$  or  $\Delta)$ -support set if there exist two orthogonal states  $\psi_0, \psi_1 \in \mathcal{H}$  (each of which is called a witness for  $S$ ) such that

- (i) the reduced density matrices of both  $\psi_0$  and  $\psi_1$  on  $\mathcal{H}_{[1,i]}$  are supported on  $\text{span } S$  (hence, the reduced density matrix of any state  $\psi \in \text{span}\{\psi_0, \psi_1\}$  on  $\mathcal{H}_{[1,i]}$  is supported on  $\text{span } S$ );
- (ii)  $|S| \leq s$ ;
- (iii) all elements in  $S$  are MPS of bond dimension at most  $b$ ;
- (iv) there are two ground states  $\Psi_0, \Psi_1 \in G$  of  $H$  such that  $|\langle \psi_0, \Psi_0 \rangle| \geq 1 - \delta$  and  $|\langle \psi_1, \Psi_1 \rangle| \geq 1 - \delta$ ; or (iv)  $\langle \psi_0, H\psi_0 \rangle \leq \epsilon_0 + \Delta\epsilon$  and  $\langle \psi_1, H\psi_1 \rangle \leq \epsilon_0 + \Delta\epsilon$  (depending on the context either  $\delta$  or  $\Delta$  is used as the precision parameter).

There are no major changes in the outline of the algorithm. Support sets  $S_i$ 's are iteratively constructed for  $i = 1, 2, \dots, n$ , and Table 4.1 illustrates the evolution of the parameters at every step in each iteration. A few lemmas in Section 4.4 should be modified, and a new lemma is added.

**Lemma 30.**  $\langle \psi, H\psi \rangle \leq \epsilon_0 + \eta\epsilon$  implies the existence of a ground state  $\Psi_0 \in G$  such that  $|\langle \psi, \Psi_0 \rangle|^2 \geq 1 - \eta$ .

**Lemma 31** ([70]).  $\langle \Psi'_0, \Psi_0 \rangle \geq 1 - \eta$  for any ground state  $\Psi_0 \in G$  of  $H$  and  $\Psi'_0 = \text{trunc}_{B_\eta} \Psi_0 / \|\text{trunc}_{B_\eta} \Psi_0\|$ , where  $B_\eta = 2^{\tilde{O}(1/\epsilon + \epsilon^{-1/4} \log^{3/4}(1/\eta))}$ .

**Lemma 32.**  $\langle \psi_0, H\psi_0 \rangle \leq \epsilon_0 + \Delta\epsilon$  and  $\langle \psi_1, H\psi_1 \rangle \leq \epsilon_0 + \Delta\epsilon$  imply  $\langle \psi, H\psi \rangle \leq \epsilon_0 + 2\Delta\epsilon / (1 - |\langle \psi_0, \psi_1 \rangle|)$  for any state  $\psi \in \text{span}\{\psi_0, \psi_1\}$ .

*Proof.* Any state  $\psi = \alpha\psi_0 + \beta\psi_1 \in \text{span}\{\psi_0, \psi_1\}$  has energy at most  $\epsilon_0 + 2\Delta\epsilon / (1 - |\langle \psi_0, \psi_1 \rangle|)$  as

$$\begin{aligned}
 1 &= \|\psi\|^2 \geq |\alpha|^2 + |\beta|^2 - 2|\alpha| \cdot |\beta| \cdot |\langle \psi_0, \psi_1 \rangle| \Rightarrow |\alpha|^2 + |\beta|^2 \leq 1 / (1 - |\langle \psi_0, \psi_1 \rangle|) \\
 &\Rightarrow \langle \psi, (H - \epsilon_0)\psi \rangle \\
 &\leq |\alpha|^2 \langle \psi_0, (H - \epsilon_0)\psi_0 \rangle + |\beta|^2 \langle \psi_1, (H - \epsilon_0)\psi_1 \rangle + 2|\alpha| \cdot |\beta| \cdot |\langle \psi_0, (H - \epsilon_0)\psi_1 \rangle| \\
 &\leq (|\alpha|^2 + |\beta|^2)\Delta\epsilon + 2|\alpha| \cdot |\beta| \sqrt{\langle \psi_0, (H - \epsilon_0)\psi_0 \rangle \cdot \langle \psi_1, (H - \epsilon_0)\psi_1 \rangle} \\
 &\leq 2(|\alpha|^2 + |\beta|^2)\Delta\epsilon.
 \end{aligned} \tag{4.23}$$

□

## Algorithm and analysis

In the  $i$ th iteration our algorithm constructs an  $(i, p_1 p_3, p_2 p_3, \Delta = c\epsilon^6)$ -support set  $S_i$  from an  $(i-1, p_1 p_3, p_2 p_3, \Delta = c\epsilon^6)$ -support set  $S_{i-1}$  returned in the  $(i-1)$ th iteration. **Extension** is trivial, and we obtain an  $(i, dp_1 p_3, p_2 p_3, \Delta = c\epsilon^6)$ -support set  $S_i^{(1)}$ . Let  $N$  be a  $\xi$ -net over the space of boundary contractions of bond dimension  $2B_{8\sqrt{c}\epsilon^2}$ .

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### Cardinality reduction convex program and bond truncation

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0. Let the variables  $\rho_0, \rho_1$  be density matrices on  $\text{span } S_i^{(1)} \otimes \mathbf{C}^{2B_{8\sqrt{c}\epsilon^2}} \subseteq \mathcal{H}_{[1,i]} \otimes \mathbf{C}^{2B_{8\sqrt{c}\epsilon^2}}$ .  
 1. For each  $X \in N$ , solve the convex program:

$$\min \text{tr}(\rho_0 H_L); \text{ s. t. } \|\text{tr}_{[1,i-1]} \rho_0 - X\|_1 \leq \xi, \quad \text{tr } \rho_0 = 1, \quad \rho_0 \geq 0. \quad (4.24)$$

2. Let  $\varphi_0 = \sum_j \varphi_{0,j} |j\rangle$  be the eigenvector of the solution  $\rho_0$  with the largest eigenvalue.  
 3. Solve the convex program:

$$\min \text{tr}(\rho_1 H_L); \text{ s. t. } \|\text{tr}_{[1,i-1]} \rho_1 - X\|_1 \leq \xi, \quad \text{tr } \rho_1 = 1, \quad \rho_1 \geq 0, \quad \langle \varphi_0, \rho_1 \varphi_0 \rangle \leq 1/4. \quad (4.25)$$

4. Let  $\varphi_1 = \sum_j \varphi_{1,j} |j\rangle$  be the eigenvector of the solution  $\rho_1$  with the largest eigenvalue.  
 5. Let  $\varphi'_0 = \sum_j \varphi'_{0,j} |j\rangle$  and  $\varphi'_1 = \sum_j \varphi'_{1,j} |j\rangle$  be the states obtained by truncating each bond (in whatever order) of  $\varphi_0$  and  $\varphi_1$  to  $p_2$ , respectively.  
 6.  $S_i^{(3)}$  consists of the MPS representations of all  $\varphi'_{0,j}, \varphi'_{1,j}$ .

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**Lemma 33** ([70]). *For any ground state  $\Psi_0 \in G$  of  $H$ ,*

$$\|(1 - P_t)\Psi_0\| \leq 100 \cdot 2^{-t/20}. \quad (4.26)$$

**Lemma 34.** *There exist two states  $\psi_0, \psi_1 \in \text{span } S_i^{(1)} \otimes \mathcal{H}_R^{\leq t}$  of Schmidt rank  $B_{8\sqrt{c}\epsilon^2}$  (across the cut  $i|i+1$ ) such that  $\langle \psi, H\psi \rangle \leq \epsilon_0 + 200c^{1/4}\epsilon$  for any state  $\psi \in \text{span}\{\psi_0, \psi_1\}$ .*

*Proof.* Let  $\phi_0 \perp \phi_1$  be two orthogonal witnesses for  $S_i^{(1)}$ . Define  $\phi'_0 = P_t \phi_0 / \|P_t \phi_0\|$ . The proof of Lemma 24 implies that the state  $\psi_0 := \text{trunc}_{B_{8\sqrt{c}\epsilon^2}} \phi'_0 / \|\text{trunc}_{B_{8\sqrt{c}\epsilon^2}} \phi'_0\|$  has energy  $\langle \psi_0, H\psi_0 \rangle \leq \epsilon_0 + 75c^{1/4}\epsilon$ . Since  $\phi_0$  is a low-energy state, Markov's inequality in probability theory implies  $|\langle \phi_0, \phi'_0 \rangle| \geq 999/1000$  for sufficiently large  $t$ . The proof of Lemma 21 implies  $|\langle \psi_0, \phi'_0 \rangle| \geq 999/1000$  for sufficiently small  $c$ . Lemma 15 implies  $|\langle \psi_0, \phi_0 \rangle| \geq 249/250$ . Similarly, we obtain another state  $\psi_1$  such that  $\langle \psi_1, H\psi_1 \rangle \leq \epsilon_0 + 75c^{1/4}\epsilon$  and  $|\langle \psi_1, \phi_1 \rangle| \geq 249/250$ . It is easy to see  $|\langle \psi_0, \psi_1 \rangle| \leq 1/5$ , and Lemma 32 implies that  $\langle \psi, H\psi \rangle \leq \epsilon_0 + 200c^{1/4}\epsilon$  for any state  $\psi \in \text{span}\{\psi_0, \psi_1\}$ .  $\square$

**Lemma 35.** *For any state  $\psi \in \text{span}\{\psi_0, \psi_1\}$ , let  $X \in N$  be the element that is closest to  $\text{cont } \psi$ . Then, at least one of the following must hold:*

- (i)  $\Phi_0 = U_\psi \varphi_0$  has energy at most  $\epsilon_0 + \epsilon/20000$  and satisfies  $|\langle \psi, \Phi_0 \rangle| \geq 1/2$ ;
- (ii)  $\Phi_0 = U_\psi \varphi_0$  and  $\Phi_1 = U_\psi \varphi_1$  have energies at most  $\epsilon_0 + \epsilon/20000$  and satisfy  $|\langle \Phi_0, \Phi_1 \rangle| \leq \sqrt{3}/2$ .



*Proof.* The proof of Lemma 25 implies that  $\sigma_0 = U_\psi \rho_0 U_\psi^{-1}$  has energy  $\text{tr}(\sigma_0 H) \leq \epsilon_0 + \epsilon/60000$  for sufficiently small  $\xi = \tilde{\Omega}(\epsilon)$  and sufficiently small constant  $c$ . We observe that (1) there exists at least an eigenstate of  $\sigma_0$  with energy at most  $\epsilon_0 + \epsilon/20000$ ; (2) there are at most two such eigenstates as Lemma 30 implies that such eigenstates are close to the ground-state space  $G$ ; (3) one of these eigenstates has the largest eigenvalue (at least  $1/3$ ) due to Markov's inequality in probability theory; (4) this eigenstate is  $\Phi_0 = U_\psi \varphi_0$ . Therefore, (i) holds if  $|\langle \psi, \Phi_0 \rangle| \geq 1/2$ . Otherwise,  $U_\psi^{-1} |\psi\rangle \langle \psi| U_\psi$  is a feasible solution to the second convex program (4.25), and the proof of Lemma 25 implies that  $\sigma_1 = U_\psi \rho_1 U_\psi^{-1}$  has energy  $\text{tr}(\sigma_1 H) \leq \epsilon_0 + \epsilon/60000$ . Let  $\Phi_1 = U_\psi \varphi_1$  be the eigenvector of  $\sigma_1$  with the largest eigenvalue  $\lambda$ . Similarly, we observe  $\lambda \geq 1/3$  and  $\langle \Phi_1, H \Phi_1 \rangle \leq \epsilon_0 + \epsilon/20000$ . Therefore, (ii) holds because  $\langle \Phi_0, \sigma_1 \Phi_0 \rangle \leq 1/4$  implies  $|\langle \Phi_0, \Phi_1 \rangle| \leq \sqrt{3}/2$ .  $\square$

*Remark.* Lemma 32 implies that  $S_i^{(2)}$  is an  $(i, p_1, dp_1 p_2 p_3^2, \Delta = 1/1000)$ -support set with  $p_1 = O(B_{8\sqrt{c}\epsilon^2} |N|) = 2^{2^{\tilde{O}(1/\epsilon)}}$ , where  $S_i^{(2)}$  consists of the MPS representations of all  $\varphi_{0,j}, \varphi_{1,j}$ .

**Lemma 36.**  $S_i^{(3)}$  is an  $(i, p_1, p_2, \delta = 1/20)$ -support set.

*Proof.*  $\Phi_k$  and  $\varphi_k$  for  $k = 0, 1$  in Lemma 35 are functions of  $\psi \in \text{span}\{\psi_0, \psi_1\}$ . We make this explicit by using the notations  $\Phi_k(\psi), \varphi_k(\psi)$ . Lemma 35 implies the existence of  $\psi, \psi' \in \text{span}\{\psi_0, \psi_1\}$  and  $k, k' \in \{0, 1\}$  such that  $\Phi_k(\psi)$  and  $\Phi_{k'}(\psi')$  have energies at most  $\epsilon_0 + \epsilon/20000$  and satisfy  $|\langle \Phi_k(\psi), \Phi_{k'}(\psi') \rangle| \leq \sqrt{3}/2$ . Let  $\varphi'_k(\psi)$  be the state obtained by truncating each bond (in whatever order) of  $\varphi_k(\psi)$  to  $p_2 = 10000n2^{\tilde{O}(\epsilon^{-1/4} \log^{3/4} n)}$ , and  $\Phi'_k(\psi)$  be the state obtained by truncating each bond to the left of the cut  $i|i+1$  (in the same order) of  $\Phi_k(\psi)$  to  $p_2$ . A minor modification of the proof of Lemma 26 implies the existence of a ground state  $\Psi_0 \in G$  such that  $|\langle \Phi'_k(\psi), \Psi_0 \rangle| \geq 999/1000$  (i.e.,  $\Phi'_k(\psi) = U_\psi \varphi'_k(\psi)$  is a witness for  $S_i^{(3)}$ ) and  $|\langle \Phi_k(\psi), \Phi'_k(\psi) \rangle| \geq 499/500$ . Similarly,  $\Phi'_{k'}(\psi') = U_{\psi'} \varphi'_{k'}(\psi')$  is another witness with  $|\langle \Phi_{k'}(\psi'), \Phi'_{k'}(\psi') \rangle| \geq 499/500$ . We obtain two orthogonal witnesses  $\Phi'_0, \Phi'_1 \in \text{span}\{\Phi'_k(\psi), \Phi'_{k'}(\psi')\}$  for  $S_i^{(3)}$  as an  $(i, p_1, p_2, \delta = 1/20)$ -support set.  $\square$

Lemmas 27, 28 imply two witnesses  $\phi'_0 = K\Phi'_0/\|K\Phi'_0\|$  and  $\phi'_1 = K\Phi'_1/\|K\Phi'_1\|$  for  $S_i$  with energies  $\langle \phi'_0, H\phi'_0 \rangle \leq \epsilon_0 + \eta\epsilon/50$  and  $\langle \phi'_1, H\phi'_1 \rangle \leq \epsilon_0 + \eta\epsilon/50$ . It is easy to see  $|\langle \phi'_0, \Phi'_0 \rangle| \geq \sqrt{3}/2$  and  $|\langle \phi'_1, \Phi'_1 \rangle| \geq \sqrt{3}/2$ . Hence  $|\langle \phi'_0, \phi'_1 \rangle| \leq \sqrt{3}/2$ , and Lemma 32 implies that any state in  $\text{span}\{\phi'_0, \phi'_1\}$  has energy at most  $\epsilon_0 + \eta\epsilon/3$ . Therefore,  $S_i$  is a support set with  $\Delta = \eta$ .

## 4.7 Frustration-free systems

It is claimed [95] that the algorithm in Lemma 12 runs in randomized polynomial time even in general non-degenerate 1D gapped systems. However, this claim does not seem to be well justified, because a possibly exponential (in  $n$ ) factor is missing in the analysis of **error reduction** in [95] if the Hamiltonian  $H = \sum_{i=1}^n H_i$  is not almost frustration-free.

We briefly recall the sampling MPO  $K$  constructed in Section 2.3.1 of [95], which reduces the precision parameter of  $S_i^{(3)}$  such that  $\delta = O(\epsilon^2/n) = \text{poly}(\epsilon/n)$  for  $S_i$ . We first define

$A = C^m(1 - H/n)^m$  with  $C = 1/(1 - \epsilon_0/n)$ . Clearly,  $A\Psi_0 = \Psi_0$  and  $\|A\Psi_1\| \leq C^m(1 - (\epsilon_0 + \epsilon)/n)^m \leq (1 - \epsilon/n)^m$  for any state  $\Psi_1 \perp \Psi_0$ . Hence, setting  $m = O(n/\epsilon) \log(n/\epsilon)$  gives  $\|A - |\Psi_0\rangle\langle\Psi_0|\| \leq \text{poly}(\epsilon/n)$ . The operator  $A$  can be expanded as a sum of an exponential number of terms:

$$A = \frac{1}{n^m} \sum_{I=(i_1, \dots, i_m) \in \{1, \dots, n\}^{\otimes m}} P_I \quad \text{with } P_I := C^m \prod_{j=1}^m (1 - H_{i_j}). \quad (4.27)$$

**Definition 11** (sampling MPO [95]). Let the sampling MPO  $K := (1/l) \sum_{j=1}^l P_{I_j}$  be the average of  $l$  terms chosen uniformly at random from all terms in the expansion of  $A$ .

**Lemma 37.** *Setting  $l = (n/\epsilon)^{O(1+\epsilon_0/\epsilon)}$  gives a sampling MPO  $K$  such that with probability at least  $1 - 1/\text{poly } n$ ,*

(a)  $\|K - A\| \leq \text{poly}(\epsilon/n)$ ;

(b) *the bond dimension of  $K$  is  $D = l2^{O(m/n)} = (n/\epsilon)^{O(1/\epsilon+\epsilon_0/\epsilon)}$ .*

*Proof sketch.* (a) is an immediate corollary of the Chernoff bound for matrices [143]:  $l = \text{poly}(n/\epsilon)C^{O(m)} = (n/\epsilon)^{O(1+\epsilon_0/\epsilon)}$ . (b) follows from a well-known fact in probability theory.  $\square$

Recall from the proof of Lemma 26 that  $\Phi'$  is a witness for  $S_i^{(3)}$  with  $|\langle\Phi', \Psi_0\rangle| \geq 19/20$ . Lemma 37(a) implies  $|\langle\phi', \Psi_0\rangle| \geq 1 - \text{poly}(\epsilon/n)$  for  $\phi' = K\Phi'/\|K\Phi'\|$  with high probability. Therefore,  $S_i$  is an  $(i, p_1D, p_2D, \delta = \text{poly}(\epsilon/n))$ -support set with probability at least  $1 - 1/\text{poly } n$ . Clearly, the bond dimension  $D = n^{O(1/\epsilon+\epsilon_0/\epsilon)}$  is a polynomial in  $n$  in almost frustration-free 1D gapped systems (i.e.,  $\epsilon_0 = O(1)$ ) but may be exponential in  $n$  in general 1D gapped systems (e.g.,  $\epsilon_0 = \Theta(n)$ ).

In frustration-free 1D gapped systems, the algorithm in Lemma 12 can be derandomized using the detectability lemma. Let  $P_i$  be the projection onto the ground-state space of  $H_i$ . Define

$$A = \prod_{\text{even } i} P_i \prod_{\text{odd } i} P_i = P_2P_4P_6 \cdots P_1P_3P_5 \cdots . \quad (4.28)$$

Clearly,  $A\Psi_0 = \Psi_0$ .

**Lemma 38** (detectability lemma [6]).  $\|A\Psi_1\| \leq (1 + \epsilon/2)^{-1/3}$  for any state  $\Psi_1 \perp \Psi_0$ .

Let  $K = A^m$  with  $m = O(1/\epsilon) \log(n/\epsilon)$  such that  $|\langle\phi', \Psi_0\rangle| \geq 1 - \text{poly}(\epsilon/n)$  for  $\phi' = K\Phi'/\|K\Phi'\|$ . Since  $A$  is an MPO of bond dimension  $d^2$ , the bond dimension of  $K$  is  $D = d^{2m} = (n/\epsilon)^{O(1/\epsilon)}$ .

## Chapter 5

# Do area laws imply efficient tensor network representations?

We show that the 2D local Hamiltonian problem with the restriction that the ground state satisfies area laws is QMA-complete. We also prove similar results in 2D translationally invariant systems and for the 3D Heisenberg and Hubbard models in external magnetic fields. Consequently, in general the ground states of local Hamiltonians satisfying area laws do not have efficient classical representations that support efficient computation of local expectation values unless QMA=NP. Conceptually, even if in the future area laws are proved for the ground state in 2D gapped systems, there is still a long way to go towards understanding the computational complexity of 2D gapped systems.

### 5.1 Introduction

Computing the ground state of local Hamiltonians is a fundamental problem in condensed matter physics. Intuitively, this problem is likely intractable because the dimension of the Hilbert space for a quantum many-body system grows exponentially with the system size. In a pioneering work [91] (see [8] for a write-up available online), Kitaev defined the complexity class QMA as the quantum analog of NP (or more precisely, the quantum analog of MA) and proved that the local Hamiltonian problem with 5-body interactions is QMA-complete. This work is followed by a line of research: The local Hamiltonian problem is QMA-complete even in (a) qubit systems with 2-body interactions [85, 111]; (b) 1D quantum systems with nearest-neighbor interactions [7, 58]; (c) 1D translationally invariant systems [84, 53] (the result of Ref. [53] is QMA<sub>EXP</sub>-complete due to a technical reason to be explained later); (d) 2D Heisenberg and Hubbard models [137] (see [17] for a summary of QMA-complete problems). Consequently, (assuming QMA≠NP) in general the ground states of local Hamiltonians do not have efficient classical representations that support efficient computation of local expectation values. Here, the first “efficient” means that the classical representation uses a polynomial number of bits, and the second “efficient” means that local expectation values

can be computed in polynomial time from the classical representation. It should be emphasized that the latter “efficient” is crucial. Indeed, (assuming non-degeneracy) the local Hamiltonian itself is an efficient classical representation of its ground state as it is the sum of a polynomial number of terms, but (assuming  $\text{QMA} \neq \text{P}$ ) this trivial representation does not support efficient computation of local expectation values.

Entanglement appears to be a central concept from an algorithmic perspective. Generic states in quantum many-body systems satisfy the volume law—the entanglement of a region scales as the number of sites inside (i.e., the volume of) the region [65]. Perhaps surprisingly, a large class of physical states satisfy the area law [40]—the entanglement of a region scales as its boundary (area). Besides its beautiful mathematical formulation, area law is gaining popularity in the emerging field of quantum Hamiltonian complexity [113, 49] because it does capture the essence of classical simulability of 1D quantum systems: Bounded (or even logarithmic divergence of) Renyi entanglement entropy across all bipartite cuts implies [146] efficient MPS representations [41, 155, 118], which underlie the celebrated DMRG algorithm [161, 162]. Since local expectation values of MPS can be computed efficiently, we conclude that the 1D local Hamiltonian problem with the restriction that the ground state satisfies area laws is in NP. Furthermore, a structural result from the proof [59, 10, 70] of the area law for the ground state of 1D gapped Hamiltonians is an essential ingredient of the (provably) polynomial-time algorithm [95, 69, 33] for computing such states, establishing that the 1D gapped Hamiltonian problem is in P.

2D quantum systems can host exotic phases of matter, and are much more exciting and challenging. Indeed, little rigorous results are known for 2D quantum systems from an algorithmic perspective. Whether area laws hold for the ground states in 2D gapped systems is one of the most well-known open problems in the field of Hamiltonian complexity. Ambitiously, one may ask (1) Which class of 2D ground states has efficient classical representations that support efficient computation of local expectation values? (2) If such classical representations exist, can we find them efficiently? A lot of effort has been devoted to extending methods and tools from 1D to 2D. Tensor network states [149] are generalizations of MPS to higher dimensions. Examples include projected entangled pair states [147] and the multi-scale entanglement renormalization ansatz [153], which, respectively, do not [138] and does [152] support efficient computation of local expectation values. It is commonly believed that physical states satisfying area laws have efficient tensor network state representations. This belief is not provable before “physical” is defined. We do not attempt to define such a notion here, but rather rely on intuitions to judge what is physical. For instance, the ground states of local Hamiltonians are more physical than generic states in quantum many-body systems, and translationally invariant Hamiltonians on a regular lattice with nearest-neighbor interactions are more physical than generic local Hamiltonians.

In contrast to the belief, it was recently proved that there exist quantum states satisfying area laws for all Renyi entanglement entropies but do not have efficient classical representations [48]. The main idea of the proof is so elegant that we would like to sketch here. The authors of Ref. [48] consider the question: How large is the space of all states satisfying area laws? They explicitly construct a set  $S$  such that (i)  $S$  is parameterized by an exponential

number of independent parameters; (ii) all states in  $S$  satisfy area laws. Consequently, a generic state in  $S$  cannot be approximated using a polynomial number of bits (as the volume of  $S$  is too large) and does not have efficient classical representations. This counting approach is very powerful: It applies to any classical representation, regardless of whether the classical representation supports efficient computation of local expectation values. We conclude that a generic state in  $S$  is not only not a tensor network state of polynomial bond dimension, but also not a (non-degenerate) eigenstate of local Hamiltonians [48].

In this chapter, we show that the 2D local Hamiltonian problem with the restriction that the ground state satisfies area laws is QMA-complete. We also prove similar results in 2D translationally invariant systems and for the 3D Heisenberg and Hubbard models with local magnetic fields. Consequently, (assuming  $\text{QMA} \neq \text{NP}$ ) in general the ground states of local Hamiltonians satisfying area laws still do not have efficient classical representations that support efficient computation of local expectation values. The result of Ref. [48] is incomparable to ours: It considers general states in quantum many-body systems while we limit ourselves to the ground states of local Hamiltonians, which are more physical. Technically, the counting approach, which is the key to the result of Ref. [48], does not work in our context. It should be emphasized that our results are not intended for diminishing the importance of area laws. A proof of (or a counterexample to) area laws for the ground state in 2D gapped systems is, in our opinion, a landmark achievement, which probably requires the development of powerful new techniques. However, even if such area laws are proved, it is just a starting point and there is still a long way to go towards understanding the computational complexity of 2D gapped systems.

## 5.2 Preliminaries

We begin with the definition of the lattice Hamiltonian problem, which is the local Hamiltonian problem tailored to the context that the Hamiltonian acts on a regular lattice with nearest-neighbor interactions (and on-site terms). Accounting for the finite precision of numerical computing, hereafter, every real number is assumed to be represented by a polynomial number of bits.

**Definition 12** (lattice Hamiltonian problem). Consider a quantum many-body system of spins (or bosons, fermions) arranged on a regular lattice. We are given a Hamiltonian  $H$  (which is the sum of nearest-neighbor interactions) and a real number  $a$  with the promise that either (Yes)  $\lambda(H) \leq a$  or (No)  $\lambda(H) \geq a + \delta$ , where  $\lambda(H)$  denotes the ground-state energy of  $H$ , and  $\delta$  is some inverse polynomial in the system size. We must decide which is the case.

QMA is the class of problems that can be efficiently verified by a quantum computer. Below is a formal definition of QMA based on quantum circuits.

**Definition 13** (QMA [91]). A problem is in QMA if there is a uniform family of polynomial-size quantum circuits  $\{V_x\}$  (one for each input instance  $x$ ) such that:

- (i) If  $x$  is a yes instance, then there exists a quantum state  $|y\rangle$  of polynomial size such that  $V_x$  accepts  $|y\rangle$  with probability greater than  $2/3$ ;
- (ii) If  $x$  is a no instance, then for any quantum state  $|y\rangle$  of polynomial size  $V_x$  accepts  $|y\rangle$  with probability less than  $1/3$ .

We switch to the definitions of the Renyi entanglement entropy and the area law.

**Definition 14** (Renyi entanglement entropy). The Renyi entanglement entropy  $S_\alpha$  ( $0 < \alpha < 1$ ) of a bipartite (pure) quantum state  $\rho_{AB}$  is defined as

$$S_\alpha(\rho_A) = (1 - \alpha)^{-1} \log \text{tr} \rho_A^\alpha, \quad (5.1)$$

where  $\rho_A = \text{tr}_B \rho_{AB}$  is the reduced density matrix. Two limits are of special interest:

$$S_0(\rho_A) := \lim_{\alpha \rightarrow 0^+} S_\alpha(\rho_A) \quad (5.2)$$

is the logarithm of the Schmidt rank, and

$$S_1(\rho_A) := \lim_{\alpha \rightarrow 1^-} S_\alpha(\rho_A) = -\text{tr}(\rho_A \log \rho_A) \quad (5.3)$$

is simply referred to as the entanglement entropy.

The entanglement entropy is the most popular entanglement measure (for pure states) in quantum information and condensed matter theory.

**Definition 15** (area law for  $S_\alpha$ ). A (pure) state on a lattice satisfies area laws if for any region  $A$ ,

$$S_\alpha(\rho_A) = O(|\partial A|), \quad (5.4)$$

where  $\rho_A$  is the reduced density matrix of the region  $A$ , and  $\partial A$  is the set of the edges of the lattice connecting the region  $A$  and its complement.

Since  $S_\alpha$  is a monotonically decreasing function of  $\alpha$ , area laws for  $S_{\alpha_1}$  are more stringent than those for  $S_{\alpha_2}$  if  $\alpha_1 < \alpha_2$ . In 1D, bounded (or even logarithmic divergence of)  $S_0$  across all bipartite cuts implies efficient exact (up to the truncation of real numbers) MPS representations [155]; bounded (or logarithmic divergence of)  $S_\alpha$  for  $0 < \alpha < 1$  across all cuts implies efficient MPS approximations [146]. See [139] for an extensive discussion of the relation between the scaling of the Renyi entanglement entropy and efficient MPS approximations in 1D quantum systems.

## 5.3 Main results

In this section, we prove our main result: The 2D lattice Hamiltonian problem with the restriction that the ground state satisfies area laws is QMA-complete. Recall that  $\lambda(\cdot)$  denotes the ground-state energy of a Hamiltonian.

**Theorem 5.** *We are given a 1D lattice Hamiltonian  $H' = \sum_{i=1}^{n-1} H'_{i,i+1}$ , where  $H'_{i,i+1}$  with  $\|H'_{i,i+1}\| \leq 1$  acts on the spins  $i$  and  $i+1$  (nearest-neighbor interaction). Then, a 2D square lattice Hamiltonian  $H$  can be efficiently constructed such that:*

- (a)  $|\lambda(H) - 2\lambda(H') - a| \leq \delta$ , where  $a$  is a real number that can be efficiently computed, and  $\delta = 1/\text{poly}(n)$  is some inverse polynomial in  $n$ ;
- (b) The ground state  $|\psi\rangle$  of  $H$  satisfies area laws for  $S_\alpha$  ( $0 < \alpha \leq 1$ );
- (c)  $H$  is translationally invariant if and only if  $H'$  is translationally invariant.

*Proof.* We construct  $H$  by stacking layers of  $H'$  so that  $H$  is translationally invariant in the direction perpendicular to the layers. We then introduce strong interlayer coupling so that  $H$  is almost trivial in the bulk. The (almost) trivial bulk “dilutes” the entanglement and implies area laws. The edges of  $H$  are nontrivial and reproduce the low-energy physics of  $H'$ .

We now give the detailed construction. Suppose  $H'$  acts on a chain of  $n$  spin- $(d/2 - 1/2)$ , i.e., the local dimension of each spin is  $d = \Theta(1)$ . Then, the Hamiltonian  $H$  acts on a 2D square lattice of size  $n \times n$ , and at each lattice site there are two spins of local dimension  $d$  (you may combine these two spins into a single spin of squared local dimension  $d^2$  if you prefer one spin per site). We label all spins by three indices  $i, j, k$  for  $1 \leq i, j \leq n$ ,  $k = 1, 2$ . The coupling between the spins  $(i, j, k)$  and  $(i', j', k')$  is denoted by  $H_{i,j,k,i',j',k'}$  which is nonzero only if  $|i - i'| + |j - j'| = 1$  (nearest-neighbor interaction). The terms within each layer are given by

$$H_{i,j,k,i+1,j,k} = H'_{i,i+1} \text{ for } 1 \leq i \leq n-1, 1 \leq j \leq n, k = 1, 2. \quad (5.5)$$

The terms between adjacent layers are given by

$$H_{i,j,2,i,j+1,1} = (\vec{S}_{i,j,2} \cdot \vec{S}_{i,j+1,1} + d^2/4 - 1/4)\Omega(n^3/\delta) \text{ for } 1 \leq i \leq n, 1 \leq j \leq n-1, \quad (5.6)$$

where  $\vec{S}_{i,j,k} = (S_{i,j,k}^x, S_{i,j,k}^y, S_{i,j,k}^z)$  is a vector of spin operators of the spin  $(i, j, k)$ , and

$$\vec{S}_{i,j,k} \cdot \vec{S}_{i',j',k'} := S_{i,j,k}^x S_{i',j',k'}^x + S_{i,j,k}^y S_{i',j',k'}^y + S_{i,j,k}^z S_{i',j',k'}^z \quad (5.7)$$

is a physical anti-ferromagnetic Heisenberg interaction. All other terms are zero. Since

$$2\vec{S}_{i,j,2} \cdot \vec{S}_{i,j+1,1} = (\vec{S}_{i,j,2} + \vec{S}_{i,j+1,1})^2 - \vec{S}_{i,j,2}^2 - \vec{S}_{i,j+1,1}^2 = (\vec{S}_{i,j,2} + \vec{S}_{i,j+1,1})^2 - (d^2 - 1)/2, \quad (5.8)$$

the ground state of  $H_{i,j,2,i,j+1,1}$  is a singlet (i.e., a state of zero total spin), and  $\lambda(H_{i,j,2,i,j+1,1}) = 0$ . Clearly, by construction  $H$  is translationally invariant in the  $j$  direction, and  $H$  is translationally invariant in the  $i$  direction if and only if  $H'$  is translationally invariant. We observe that  $H$  is the sum of  $n+1$  terms with pairwise disjoint supports. Specifically, let  $H = \sum_{j=0}^n H_j$ , where on the edges  $j = 0, n$ ,

$$H_0 = \sum_{i=1}^{n-1} H_{i,1,1,i+1,1,1} \text{ and } H_n = \sum_{i=1}^{n-1} H_{i,n,2,i+1,n,2} \quad (5.9)$$

act, respectively, on the spins  $(i, 1, 1)$  and on the spins  $(i, n, 2)$  for  $1 \leq i \leq n$ ; in the bulk  $1 \leq j \leq n - 1$ ,

$$H_j = \sum_{i=1}^{n-1} (H_{i,j,2,i+1,j,2} + H_{i,j+1,1,i+1,j+1,1}) + \sum_{i=1}^n H_{i,j,2,i,j+1,1} \quad (5.10)$$

acts on the spins  $(i, j, 2)$  and  $(i, j + 1, 1)$  for  $1 \leq i \leq n$ . Hence the ground state  $|\psi\rangle = \bigotimes_{j=0}^n |\psi_j\rangle$  of  $H$  is a product state in the  $j$  direction, where  $|\psi_j\rangle$  is the ground state of  $H_j$ .

We now bound the Renyi entanglement entropy of  $|\psi\rangle$ . For the ease of presentation, we assume the region  $A$  is rectangular. However, it should be clear that area laws hold for an arbitrary region  $A$ . Since  $|\psi\rangle = \bigotimes_{j=0}^n |\psi_j\rangle$  is a product state and the Renyi entropy is additive, we can evaluate the Renyi entanglement entropy of each  $|\psi_j\rangle$  and sum them up. Suppose the rectangular region  $A$  consists of all spins  $(i, j, k)$  with indices  $i_1 \leq i \leq i_2$ ,  $j_1 \leq j \leq j_2$ ,  $k = 1, 2$ . Then,

- (i) the Renyi entanglement entropy of  $|\psi_j\rangle$  for  $j \leq j_1 - 2$  or  $j \geq j_2 + 1$  is exactly zero because such  $|\psi_j\rangle$ 's do not intersect with the boundary of  $A$ ;
- (ii) the Renyi entanglement entropy of  $|\psi_j\rangle$  for  $j = j_1 - 1$  or  $j = j_2$  is trivially upper bounded by  $O(i_2 - i_1)$ ;
- (iii) the Renyi entanglement entropy of  $|\psi_j\rangle$  for each  $j_1 \leq j \leq j_2 - 1$  is  $O(1)$ . This is a straightforward consequence of the area law for the ground state in 1D gapped systems.

**Lemma 39** ([70]). *Let  $|\Psi\rangle$  be the ground state of the 1D lattice Hamiltonian  $\mathbf{H} = \sum_{i=1}^{n-1} \mathbf{H}_{i,i+1}$ , where  $\mathbf{H}_{i,i+1}$  with  $\|\mathbf{H}_{i,i+1}\| \leq 1$  acts on the spins  $i$  and  $i + 1$  (nearest-neighbor interaction). Suppose the energy gap (i.e., the difference between the smallest and the second smallest eigenvalues) of  $\mathbf{H}$  is  $\Theta(1)$ . Then, the Renyi entanglement entropy  $S_\alpha(0 < \alpha \leq 1)$  of  $|\Psi\rangle$  is  $O(1)$  per cut.*

Case (iii) follows from this lemma by noting that  $|\psi_j\rangle$  is the ground state of  $H_j$ , which becomes a 1D lattice Hamiltonian by combining the spins  $(i, j, 2)$  and  $(i, j + 1, 1)$  into a single spin for each  $1 \leq i \leq n$ . Indeed, after rescaling  $H_j$  so that the norm of each term in  $H_j$  is  $O(1)$ , we observe that its energy gap is  $\Omega(1)$ . Summing up cases (i) (ii) (iii), we obtain the upper bound  $O(i_2 - i_1 + j_2 - j_1)$ , i.e., a 2D area law for the Renyi entanglement entropy  $S_\alpha(0 < \alpha \leq 1)$ .

We now estimate  $\lambda(H)$ . Since  $H = \sum_{j=0}^n H_j$  and the supports of  $H_j$ 's are pairwise disjoint,

$$\lambda(H) = \sum_{j=0}^n \lambda(H_j) = 2\lambda(H') + (n - 1)\lambda(H_1), \quad (5.11)$$

where the second step is due to  $\lambda(H_0) = \lambda(H_n) = \lambda(H')$  and the translational invariance in the  $j$  direction in the bulk.  $\lambda(H_1)$  can be estimated using the projection lemma.

**Lemma 40** (projection lemma [85]). *Let  $\mathbf{H}_1, \mathbf{H}_2$  be two Hamiltonians acting on the Hilbert space  $\mathcal{H} = \mathcal{H}^\parallel \oplus \mathcal{H}^\perp$ . Suppose  $\mathbf{H}_2|_{\mathcal{H}^\parallel} = 0$  and  $\mathbf{H}_2|_{\mathcal{H}^\perp} \geq J > 2\|\mathbf{H}_1\|$ , where  $\mathbf{H}_2|_{\dots}$  is the*



restriction of  $\mathbf{H}_2$  to some subspace. Then,

$$\lambda(\mathbf{H}_1|_{\mathcal{H}^\parallel}) - \|\mathbf{H}_1\|^2/(J - 2\|\mathbf{H}_1\|) \leq \lambda(\mathbf{H}_1 + \mathbf{H}_2) \leq \lambda(\mathbf{H}_1|_{\mathcal{H}^\parallel}). \quad (5.12)$$

In our context, we set

$$H_1 = \mathbf{H}_1 + \mathbf{H}_2 \text{ with } \mathbf{H}_1 = \sum_{i=1}^{n-1} (H_{i,1,2,i+1,1,2} + H_{i,2,1,i+1,2,1}) \text{ and } \mathbf{H}_2 = \sum_{i=1}^n H_{i,1,2,i,2,1}. \quad (5.13)$$

Since the supports of  $H_{i,1,2,i,2,1}$ 's are pairwise disjoint,  $\lambda(\mathbf{H}_2) = \sum_{i=1}^n \lambda(H_{i,1,2,i,2,1}) = 0$ , and the ground state  $|\phi\rangle$  of  $\mathbf{H}_2$  is a product of singlets (unique).  $\mathcal{H}^\parallel$  is the 1D subspace spanned by  $|\phi\rangle$ , and  $J = \Omega(n^3/\delta)$  is the energy gap of  $\mathbf{H}_2$ . Since  $\|\mathbf{H}_1\| = O(n)$ ,

$$\begin{aligned} \lambda(\mathbf{H}_1|_{\mathcal{H}^\parallel}) &= \langle \phi | \mathbf{H}_1 | \phi \rangle \Rightarrow |\lambda(H_1) - \langle \phi | \mathbf{H}_1 | \phi \rangle| \leq \|\mathbf{H}_1\|^2/(J - 2\|\mathbf{H}_1\|) = O(n^2/J) = \delta/n \\ &\Rightarrow |\lambda(H) - 2\lambda(H') - a| \leq \delta(n-1)/n \leq \delta \text{ for } a := (n-1)\langle \phi | \mathbf{H}_1 | \phi \rangle. \end{aligned} \quad (5.14)$$

Finally,  $a$  can be efficiently computed as  $|\phi\rangle$  is a product of singlets: The running time is  $O(n)$  if  $H'$  is not translationally invariant and  $O(1)$  if  $H'$  is.  $\square$

The construction in the proof of Theorem 5 does not imply area laws for  $S_0$  because the bulk of  $H$  is only almost trivial but not completely trivial. Practically, this is not a limitation as  $S_0$  (the logarithm of the Schmidt rank) is not continuous and hence not stable with respect to infinitesimal perturbations. In the absence of (c) translational invariance, one can easily construct a completely trivial bulk and area laws for  $S_0$  follow.

The state-of-the-art QMA-completeness result for the 1D lattice Hamiltonian problem is due to Hallgren et al. [58], which is an improvement over a previous work [7].

**Lemma 41** ([58]). *The 1D lattice Hamiltonian problem (with spin-7/2) is QMA-complete.*

**Corollary 1.** *The 2D square lattice Hamiltonian problem with the restriction that the ground state satisfies area laws for  $S_\alpha$  ( $0 \leq \alpha \leq 1$ ) is QMA-complete.*

*Proof.* This is an immediate consequence of Theorem 5 and Lemma 41. Note that Theorem 5(b) also holds for  $S_0$  in the absence of translational invariance.  $\square$

Translational invariance is an important physical condition, but from a theoretical perspective it introduces a slight technical complication that we have to address. Usually the computational complexity of a problem is measured with respect to the input size, e.g., a problem is in P if it can be solved in time growing polynomially with the input size. For non-translationally invariant local Hamiltonians, the input size is a polynomial in the system size (as a polynomial number of terms need to be specified), and hence we may equally use the system size to measure the computational complexity. For translationally invariant local Hamiltonians, however, the input size is the logarithm of the system size (the number of bits to represent the system size), and hence in this case an exponential-time algorithm (with

respect to the input size) is “efficient” in the sense that its running time grows polynomially with the system size.

For translationally invariant lattice Hamiltonians, the notion of hardness is  $\text{QMA}_{\text{EXP}}$ -complete, which for brevity we do not formally define here. Serious readers should go to the original reference [53] for its definition based on quantum Turing machines. Colloquially,  $\text{QMA}_{\text{EXP}}$ -complete (with respect to the input size) means QMA-complete with respect to the system size. This “definition” is of course imprecise, but you do not lose any conceptual messages in the following if you use it.

**Lemma 42** ([53]). *The 1D translationally invariant lattice Hamiltonian problem is  $\text{QMA}_{\text{EXP}}$ -complete.*

**Corollary 2.** *The 2D translationally invariant square lattice Hamiltonian problem with the restriction that the ground state satisfies area laws for  $S_\alpha (0 < \alpha \leq 1)$  is  $\text{QMA}_{\text{EXP}}$ -complete.*

*Proof.* This is an immediate consequence of Theorem 5 and Lemma 42.  $\square$

## 5.4 Further extensions

In this section, we extend previous results to 3D Heisenberg and Hubbard models with local magnetic fields, which are more physical than generic lattice Hamiltonians.

**Lemma 43** ([137]). *The 2D square lattice spin-1/2 Heisenberg Hamiltonian*

$$H' = \sum_{\langle i', j' \rangle} \vec{\sigma}_{i'} \cdot \vec{\sigma}_{j'} - \sum_{i'} \vec{h}_{i'} \cdot \vec{\sigma}_{i'} \quad (5.15)$$

*is QMA-complete, where  $\langle i', j' \rangle$  denotes nearest neighbors, and  $\vec{\sigma}_{i'} = (\sigma_{i'}^x, \sigma_{i'}^y, \sigma_{i'}^z)$  is a vector of Pauli matrices at site  $i'$ .*

**Proposition 1.** *The 3D cubic lattice spin-1/2 Heisenberg Hamiltonian*

$$H = \sum_{\langle i, j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - \sum_i \vec{h}_i \cdot \vec{\sigma}_i \quad (5.16)$$

*with the restriction that the ground state satisfies area laws for the entanglement entropy is QMA-complete.*

*Proof.* Given a 2D Hamiltonian (5.15), a 3D Hamiltonian (5.16) can be efficiently constructed such that:

- (a)  $|\lambda(H) - \lambda(H') + a| \leq \delta$ , where  $a$  is a real number that can be efficiently computed, and  $\delta$  is some inverse polynomial in  $n$ ;
- (b) The ground state  $|\psi\rangle$  of  $H$  satisfies area laws for the entanglement entropy.

Then, Proposition 1 is an immediate consequence of Lemma 43.

We label a site  $i'$  in the 2D square lattice by two indices  $i' = (i'_x, i'_y)$  and a site  $i$  in the 3D cubic lattice by three indices  $i = (i_x, i_y, i_z)$ , where  $1 \leq i'_x, i'_y, i_x, i_y, i_z \leq n$ . The field strengths in (5.15) are upper bounded by a fixed polynomial in  $n$  [137]:  $|\vec{h}_{i'}| \leq p(n) = \text{poly}(n)$  for any  $i'$ . The site-dependent magnetic fields in (5.16) are given by

$$\vec{h}_i = \vec{h}'_{(i_x, i_y)} + (0, 0, 1) \text{ for } i_z = 1, \text{ and } \vec{h}_i = (0, 0, n^4 p^2 / \delta) \text{ for } 2 \leq i_z \leq n. \quad (5.17)$$

$\lambda(H)$  can be estimated using the projection lemma. In our context, we set

$$\mathbf{H}_1 = \sum_{\langle i, j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - \sum_{i_x, i_y=1}^n \vec{h}_{(i_x, i_y, 1)} \cdot \vec{\sigma}_{(i_x, i_y, 1)} \text{ and } \mathbf{H}_2 = (n-1)n^6 p^2 / \delta - \sum_{i_x, i_y=1}^n \sum_{i_z=2}^n \vec{h}_i \cdot \vec{\sigma}_i \quad (5.18)$$

such that  $H = \mathbf{H}_1 + \mathbf{H}_2 - (n-1)n^6 p^2 / \delta$ . Clearly,  $\lambda(\mathbf{H}_2) = 0$ , and

$$\mathcal{H}^\parallel = \text{span}\{|\phi\rangle : \langle \phi | \sigma_i^z | \phi \rangle = 1, \forall 1 \leq i_x, i_y \leq n, 2 \leq i_z \leq n\} \text{ with } \dim \mathcal{H}^\parallel = 2^n \quad (5.19)$$

is the ground-state space of  $\mathbf{H}_2$ . Let  $J = \Omega(n^4 p^2 / \delta)$  be the smallest nonzero eigenvalue of  $\mathbf{H}_2$ . Since  $\|\mathbf{H}_1\| = O(n^2 p)$ ,

$$\begin{aligned} \lambda(\mathbf{H}_1|_{\mathcal{H}^\parallel}) &= \lambda(H') + 3n^3 - 6n^2 + 2n \Rightarrow |\lambda(H) - \lambda(H') + a| \\ &\leq \|\mathbf{H}_1\|^2 / (J - 2\|\mathbf{H}_1\|) \leq \delta \text{ for } a := (n-1)n^6 p^2 / \delta - 3n^3 + 6n^2 - 2n. \end{aligned} \quad (5.20)$$

We now bound the entanglement entropy of  $|\psi\rangle$ . Let  $P$  be the projection onto the subspace  $\mathcal{H}^\parallel$ . Since  $|\psi\rangle$  is also the ground state of  $\mathbf{H}_1 + \mathbf{H}_2$ ,

$$\begin{aligned} \|\mathbf{H}_1\| &= \|\mathbf{H}_1\| + \lambda(\mathbf{H}_2) \geq \lambda(\mathbf{H}_1 + \mathbf{H}_2) = \langle \psi | (\mathbf{H}_1 + \mathbf{H}_2) | \psi \rangle = \langle \psi | \mathbf{H}_1 | \psi \rangle + \langle \psi | \mathbf{H}_2 | \psi \rangle \\ &\Rightarrow O(n^2 p) = 2\|\mathbf{H}_1\| \geq \langle \psi | \mathbf{H}_2 | \psi \rangle = \langle \psi | (1 - P) \mathbf{H}_2 (1 - P) | \psi \rangle \geq \Omega(n^4 p^2 / \delta) \|(1 - P)|\psi\rangle\|^2 \\ &\Rightarrow \|(1 - P)|\psi\rangle\|^2 = O(n^{-2} p^{-1} \delta) \Rightarrow \|\psi - |\phi\rangle\| = 1 / \text{poly}(n) \end{aligned} \quad (5.21)$$

for  $|\phi\rangle = P|\psi\rangle / \|P|\psi\rangle\|$ . Clearly,  $|\phi\rangle \in \mathcal{H}^\parallel$  satisfies area laws for any region  $A$ . Therefore,  $|\psi\rangle$  also satisfies area laws due to the continuity of the entanglement entropy [107].  $\square$

**Lemma 44** ([137]). *The 2D square lattice (fermionic) Hubbard Hamiltonian*

$$H = - \sum_{\langle i, j \rangle, s} a_{i, s}^\dagger a_{j, s} + U \sum_i a_{i, \uparrow}^\dagger a_{j, \uparrow} a_{i, \downarrow}^\dagger a_{j, \downarrow} - \sum_i \vec{h}_i \cdot \vec{\sigma}_i \quad (5.22)$$

at half filling is QMA-complete, where  $a_{i, s}^\dagger, a_{i, s}$  are the creation and annihilation operators of spin  $s \in \{\uparrow, \downarrow\}$  at site  $i$ , and  $\vec{\sigma}_i = \sum_{s, s'} (\sigma_{ss'}^x, \sigma_{ss'}^y, \sigma_{ss'}^z) a_{i, s}^\dagger a_{i, s'}$  is a vector of operators with  $\sigma_{ss'}$  the elements of the Pauli matrices.

**Proposition 2.** *The 3D cubic lattice (fermionic) Hubbard Hamiltonian*

$$H = - \sum_{\langle i, j \rangle, s} a_{i, s}^\dagger a_{j, s} + U \sum_i a_{i, \uparrow}^\dagger a_{j, \uparrow} a_{i, \downarrow}^\dagger a_{j, \downarrow} - \sum_i \vec{h}_i \cdot \vec{\sigma}_i \quad (5.23)$$

at half filling with the restriction that the ground state satisfies area laws for the entanglement entropy is QMA-complete.

*Proof.* Proposition 2 can be proved in the same way as Proposition 1.  $\square$

## Chapter 6

# Entanglement of excited eigenstates in random spin chains

Entanglement properties of excited eigenstates (or of thermal mixed states) are difficult to study with conventional analytical methods. We approach this problem for random spin chains using a recently developed real-space renormalization group technique for excited states (“RSRG- $X$ ”). For the random  $XX$  and quantum Ising chains, which have logarithmic divergences in the entanglement entropy of their (infinite-randomness) critical ground states, we show that the entanglement entropy of excited eigenstates retains a logarithmic divergence while the mutual information of thermal mixed states does not. However, in the  $XX$  case the coefficient of the logarithmic divergence extends from the universal ground-state value to a universal interval due to the degeneracy of excited eigenstates. These models are noninteracting in the sense of having free-fermion representations, allowing strong numerical checks of our analytical predictions.

### 6.1 Introduction

Concepts from quantum information theory have been widely used in condensed matter and atomic physics [9, 40] to characterize quantum correlations in various interesting classes of states. One such concept is quantum entanglement [122, 67], which for critical ground states [66, 154, 96, 97, 28, 27], topological phases [92, 98, 99], and Fermi liquids [164, 50] provides unique insights into the physics that are difficult to obtain via other quantities. Entanglement is also quantitatively related to the difficulty of describing 1D noncritical [59, 10, 70] and critical (“finite-entanglement scaling” [142, 123, 121]) ground states by MPS [41, 118] in numerical approximations [146, 139].

In this chapter, we study random spin chains, where entanglement is known to capture important aspects of the ground state [129, 128], and examine how the entanglement of individual excited eigenstates is different from the mutual information of thermal mixed states at nonzero temperature. This question can be viewed as an entanglement version of

the classical problem of equivalence of ensembles: Is the canonical ensemble described by the density matrix  $\rho = \exp(-H/T)$ , where  $H$  is the Hamiltonian and  $T$  is the temperature, equivalent for important observables to the microcanonical ensemble of energy eigenstates with the same energy density? As  $\rho$  is a mixed state, we need a notion that generalizes the entanglement entropy (well defined only for pure states), and mutual information (though not an entanglement measure) is a commonly used option.

Another motivation for studying excited eigenstates in random spin chains is the high level of current interest [16, 110, 116, 15, 158] in how disorder (modeled by randomness) can lead to localized states violating the eigenstate thermalization hypothesis, even in the presence of interactions; this phenomenon is known as many-body localization. The eigenstate thermalization hypothesis [37, 141, 130] is that (for some not yet delineated classes of quantum many-body systems) local measurements of an energy eigenstate approach those of the thermal mixed state with the same energy density. Intuitively, one region of the system sees the rest of the system as a bath or reservoir capable of providing energy and particles. Localization does not support the transport of energy or particles and hence prevents full thermalization. We emphasize that many-body localization is a property associated with all eigenstates (not just the ground state) of disordered systems.

Excited eigenstates are “physical” states participating in the dynamics of the system, and hence their singularities strongly suggest a dynamical quantum phase transition. For example, in the random quantum Ising chain we find that the entanglement of (almost) all eigenstates becomes singular (i.e., diverges logarithmically) at the critical point. This is indeed accompanied with a dynamical quantum phase transition characterized by the time evolution of entanglement entropy [157].

The real-space renormalization group (RSRG) [102, 36, 47, 46, 45, 82] is a standard technique for “infinite-randomness” ground states in random spin chains. It has recently been generalized to excited states with the acronym RSRG-X [117]. Adapting this approach to our context, we make analytical predictions for the scaling of excited-state entanglement (defined as the average entanglement entropy of energy eigenstates sampled from a canonical ensemble) and thermal mutual information (the mutual information of a thermal mixed state) in the random  $XX$  and quantum Ising chains, which are verified numerically.

We find that excited-state entanglement and thermal mutual information behave very differently. The latter behaves as one might expect for physical quantities at nonzero temperatures above a (random) quantum critical point: The characteristic divergence [129] is cut off by temperature. The former retains such a divergence, i.e., the entanglement entropy of excited eigenstates diverges logarithmically as that of the ground state does. There is a surprise: In the random  $XX$  chain, the coefficient of the logarithmic divergence extends from the universal ground-state value to a universal interval due to the degeneracy of excited eigenstates (it is basis dependent and is determined only after a way of lifting the degeneracy of excited eigenstates is given).

Recently, we became aware of a paper [127] that studies the entanglement of states with a small finite number of excitations. It should be clear that we study the entanglement of states with a finite energy density above the ground state, i.e., an infinite number of

excitations in the thermodynamic limit.

## 6.2 Preliminaries

We start by introducing key definitions and then review RSRG. Entanglement reflects a remarkable fact about the product structure of the Hilbert space for a bipartite quantum system  $AB$ . This Hilbert space is constructed as the tensor product of the Hilbert spaces for the two subsystems, i.e., it is spanned by product states made from (basis) vectors of  $A$  and  $B$ . However, the superposition principle allows linear combinations of product states, and in general such a linear combination is not a product of any wave functions in  $A$  and  $B$ .

The entanglement entropy of a pure state  $\rho_{AB}$  is the von Neumann entropy  $S(\rho_A) = -\text{tr}\rho_A \ln \rho_A$  of the reduced density matrix  $\rho_A = \text{tr}_B \rho_{AB}$ . It is the standard measure of entanglement for pure states. For mixed states, there are some entanglement measures in the literature and no single one is standard [122, 67]. Most of these entanglement measures reduce for pure states to entanglement entropy, and are difficult (NP-hard [71]) to compute. Quantum mutual information  $I(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$  is not an entanglement measure, as it is generically nonzero for separable (i.e., unentangled) states. It quantifies the total (classical and quantum) correlation between  $A$  and  $B$  in a possibly mixed state  $\rho_{AB}$ , and is the quantum analog of mutual information (the standard measure of correlation between two random variables) in classical information theory.

Let  $S_L(|\psi\rangle)$  be the entanglement entropy of the state  $|\psi\rangle$  in a spin model, where  $A$  consists of a block of  $L$  spins, and by default  $|\psi\rangle$  is the ground state.  $S_L$  satisfies an area law [40] in 1D gapped systems [59, 10, 70]. In 1D gapless systems,  $S_L \sim (c \ln L)/3$  [66, 28, 27] if the critical theory is a conformal field theory with central charge  $c$ , e.g.,  $S_L \sim (\ln L)/3$  in the homogeneous  $XX$  and anti-ferromagnetic Heisenberg chains [154, 96, 97]. Similarly, let  $I_L^T$  be the mutual information of the thermal mixed state  $\exp(-H/T)$  at nonzero temperature  $T$ .  $I_L^T$  always satisfies an area law [165], regardless of the energy gap or the dimension (geometry) of the lattice.

## 6.3 Methods

As a standard analytical approach to the low-energy physics in random spin chains, RSRG is successful in practice and believed to be asymptotically exact at infinite-randomness quantum critical points. We briefly illustrate this approach in the context of the random  $XX$  chain [46]. See Ref. [82] and references therein for details and more examples.

The Hamiltonian is  $H = \sum_i H_i$  with  $H_i = J_i(\sigma_x^i \sigma_x^{i+1} + \sigma_y^i \sigma_y^{i+1})$ , where  $J_i$ 's are independent and identically distributed (i.i.d.) random variables. At each step of RSRG, we find the strongest bond  $J_j = \max_i J_i =: \Omega$  and diagonalize  $H_j$ . Assuming  $J_j \gg J_{j\pm 1}$ , the spins  $j$  and  $j + 1$  form a singlet (the ground state of  $H_j$ ), and then degenerate perturbation theory

Table 6.1: Eigenvalues and eigenstates of  $H_j$ ; effective interactions  $H_{j-1,j+2} = J_{j-1,j+2}(\sigma_x^{j-1}\sigma_x^{j+2} + \sigma_y^{j-1}\sigma_y^{j+2})$ .

Eigenvalues	Eigenstates	Effective interactions
$2J_j$	$ \uparrow_j\downarrow_{j+1}\rangle +  \downarrow_j\uparrow_{j+1}\rangle$	$J_{j-1,j+2} = J_{j-1}J_{j+1}/J_j$
0	$ \uparrow_j\uparrow_{j+1}\rangle,  \downarrow_j\downarrow_{j+1}\rangle$	$J_{j-1,j+2} = -J_{j-1}J_{j+1}/J_j$
$-2J_j$	$ \uparrow_j\downarrow_{j+1}\rangle -  \downarrow_j\uparrow_{j+1}\rangle$	$J_{j-1,j+2} = J_{j-1}J_{j+1}/J_j$

(Schrieffer-Wolff transformation [25]) leads to an effective interaction

$$J_{j-1,j+2} = J_{j-1}J_{j+1}/J_j < \Omega \quad (6.1)$$

between the spins  $j - 1$  and  $j + 2$ . As such, we eliminate the strongest bond  $J_j$  and reduce the energy scale  $\Omega$ . Repeating these steps, the ground state of the random  $XX$  chain is approximately a tensor product of singlets. Moreover, Eq. (6.1) induces a RSRG flow equation for the distribution of  $J_i$ 's. There is a simple infinite-randomness fixed point solution as the attractor for all nonsingular initial distributions of  $J_i$ 's [46], which justifies the assumption  $J_j \gg J_{j\pm 1}$  in the asymptotic limit. Therefore, the low-energy physics of the random  $XX$  chain is universal: It is governed by the fixed point distribution, regardless of initial distributions.

The entanglement entropy  $S_L$  is proportional to the number of singlets across one boundary of the block [129]. Let  $\Gamma = \ln(\Omega_0/\Omega)$  with  $\Omega_0$  the initial energy scale. The RSRG flow equation and the fixed point distribution imply (a)  $\lambda \sim \Gamma^2$ , where  $\lambda$  is the length scale of the singlets at the energy scale  $\Omega$ , and (b)  $N \sim (\ln \Gamma)/3$ , where  $N$  is the average total number of singlets across a particular cut at energy scales greater than  $\Omega$ . Substituting  $\lambda \sim L$ ,

$$\langle S_L \rangle \sim 2N \ln 2 \sim (\ln 2)(\ln L)/3, \quad (6.2)$$

where  $\langle \cdot \rangle$  denotes averaging over randomness. See Refs. [129, 128] for details.

In free-fermion systems, the algorithm for computing entanglement entropy is well established [120]. It is used in Refs. [154, 96, 94] to compute the entanglement entropy of ground states in the homogeneous (and random)  $XX$  chain, quantum Ising chain, etc., and it also works for excited eigenstates. The algorithm for computing the mutual information of thermal states is a variant of it [120]. Technically, these algorithms make use of (i) the fact that a free-fermion system can be decomposed into a bunch of noninteracting fermionic modes, and (ii) the observation that the eigenstates and the thermal states of a free-fermion Hamiltonian are (fermionic) Gaussian states, i.e., they can be reconstructed from their covariance matrices. Since these algorithms are efficient in the sense that their running time grows polynomially with the system size, we are able to simulate chains of 200–1000 spins with a laptop and extract the coefficient of “ $\ln L$ ” convincingly. We verify with accurate numerics all implications of RSRG and RSRG-X for the scaling of excited-state entanglement and thermal mutual information. This is a numerical test of the recently developed RSRG-X [117].

## 6.4 Random $XX$ chain

Let  $\{|\psi_i\rangle\}$  be a complete set of eigenstates of  $H$ , and define

$$S_L^T = \frac{\sum_i \exp(-\langle \psi_i | H | \psi_i \rangle / T) S_L(|\psi_i\rangle)}{\sum_i \exp(-\langle \psi_i | H | \psi_i \rangle / T)} \quad (6.3)$$

as the average entanglement entropy of eigenstates  $|\psi_i\rangle$ 's sampled from the Boltzmann distribution at temperature  $T$ . Here  $T$  is a parameter tuning the (average) energy, for we wonder whether (and how) the scaling of excited-state entanglement depends on energy. Alternatively, one may study the average entanglement entropy of eigenstates with (close to) a particular energy. Note that  $S_L^T$  is not the entanglement of the thermal mixed state  $\exp(-H/T)$ .

RSRG-X [117] is an approach to the long-range physics of excited states in random spin chains. Following our previous discussion of RSRG, we show implications of RSRG-X for the scaling of  $\langle S_L^T \rangle$  in the random  $XX$  chain.

At each step of RSRG-X, we still diagonalize  $H_j$ : The eigenvalues and eigenstates are given in Table 6.1. Here the spins  $j$  and  $j+1$  are in a random eigenstate of  $H_j$  sampled from the Boltzmann distribution at temperature  $T$  (cf. they are always in the ground state of  $H_j$  in RSRG), and then degenerate perturbation theory leads to an effective interaction between the spins  $j-1$  and  $j+2$ : Different eigenstates may induce different interactions, but fortunately the difference is only in sign. Hence the flow equation and the fixed point solution for the distribution of  $|J_i|$ 's in RSRG-X are identical to those in RSRG.

We calculate the amount of entanglement generated in RSRG-X. (i) If the spins  $j$  and  $j+1$  are in an eigenstate of  $H_j$  with eigenvalue  $\pm 2J_j$ , then a unit of entanglement is generated as in RSRG. (ii) Otherwise, the spins  $j$  and  $j+1$  may be in a superposition of  $|\uparrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$ , and an undetermined amount of entanglement is generated. Let  $\alpha$  be the ratio of the amount of entanglement generated in RSRG-X to that generated in RSRG. Averaging cases (i) and (ii) gives  $1/2 \leq \alpha \leq 1$ . At any constant temperature  $T > 0$ , the energy scale  $\Omega$  becomes much lower than  $T$  after some number of RSRG-X steps. Hence the scaling of  $\langle S_L^{T>0} \rangle$  is the same as that of  $\langle S_L^{T=\infty} \rangle$ . Summarizing,

$$\langle S_L^{T=\infty} \rangle \sim \langle S_L^{T>0} \rangle \sim \alpha (\ln 2)(\ln L)/3, \quad 1/2 \leq \alpha \leq 1. \quad (6.4)$$

It is not a limitation of our approach that the prefactor  $\alpha$  is undetermined. Indeed, the eigenvalues of a random  $XX$  Hamiltonian are degenerate. Hence the complete set of eigenstates  $\{|\psi_i\rangle\}$  and the scaling of  $\langle S_L^T \rangle$  are not unique. We construct two examples in which  $\alpha = 1/2$  and  $\alpha = 1$ , respectively.

**Example 1.** Since the total magnetization  $\sigma_z = \sum_i \sigma_z^i$  is conserved, one may require that each  $|\psi_i\rangle$  is an eigenstate of  $\sigma_z$ , which is physically interpreted as fixing the fermion number in the fermion representation. Then, in case (ii) the spins  $j$  and  $j+1$  are (approximately) in either  $|\uparrow\uparrow\rangle$  or  $|\downarrow\downarrow\rangle$  (not a superposition) so that (almost) no entanglement is generated.



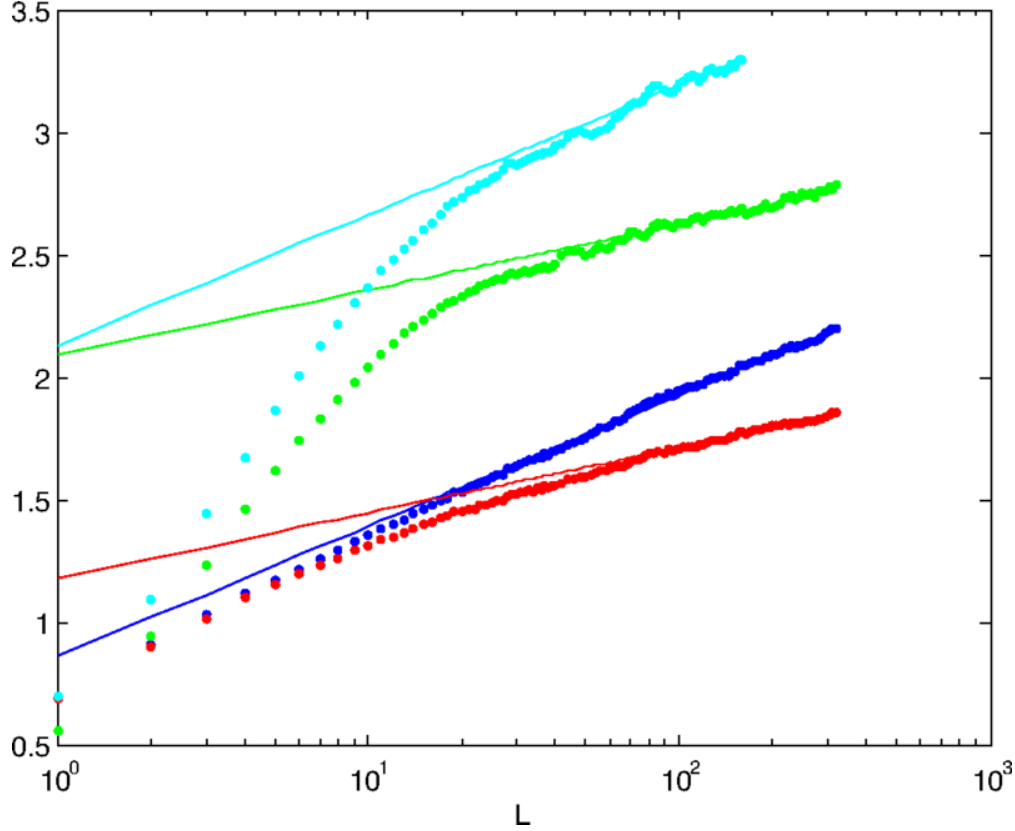


Figure 6.1: (Color online) Scaling of  $\langle S_L^T \rangle$  in random  $XX$  chain. Here  $J_i$ 's are i.i.d. uniform random variables on the interval  $[0, 1]$ . Example 1 ( $\alpha = 1/2$ ). The blue, red, and green dots are data (averaged over 5000 samples) for  $T = 0, 10^{-3}$ , and  $\infty$ , respectively, in chains of 1000 spins. The lines are fits based on (6.2) and (6.4):  $(\ln 2)(\ln L)/3 + 0.86$  (blue),  $(\ln 2)(\ln L)/6 + 1.18$  (red), and  $(\ln 2)(\ln L)/6 + 2.09$  (green). Example 2 ( $\alpha = 1$ ). The cyan dots are data (averaged over 3000 samples) for  $T = \infty$ ,  $\delta = 10^{-9}$  in chains of 500 spins. The cyan line is a fit based on (6.4):  $(\ln 2)(\ln L)/3 + 2.13$ .

Hence  $\alpha = 1/2$ , which is verified numerically for  $T = \infty$  (green) and  $T = 10^{-3}$  (red) in Fig. 6.1. Note that the (universal) logarithmic scaling starts at larger  $L$  for  $T = 10^{-3}, \infty$  than for  $T = 0$  (blue).

**Example 2.** Let  $H' = \sum_i (1 + \delta) J_i \sigma_x^i \sigma_x^{i+1} + J_i \sigma_y^i \sigma_y^{i+1}$  such that  $\lim_{\delta \rightarrow 0} H' = H$ . The eigenvalues of  $H'$  are generically non-degenerate. Then, in case (ii) the spins  $j$  and  $j + 1$  are (approximately) in  $(|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle)/\sqrt{2}$  (maximally entangled state) so that (almost) one unit of entanglement is generated. Hence  $\alpha = 1$ , which is verified numerically for  $T = \infty$  (cyan) in Fig. 6.1.

We calculate the scaling of  $\langle I_L^T \rangle$  using RSRG. (i) If  $\Omega \gg T$ , we do RSRG as if  $T = 0$ .

(ii) If  $\Omega \ll T$ , the remaining spins are in the maximally mixed state as if  $T = \infty$ . (iii) The transition occurs at  $\Omega_c \sim T$ :

$$L_c \sim \Gamma_c^2 \sim \ln^2(1/\Omega_c) \sim \ln^2(1/T). \quad (6.5)$$

The thermal mixed state  $\exp(-H/T)$  is approximately of the form  $\rho_1 \otimes \rho_0$ , where  $\rho_1$  is a tensor product of singlets, and  $\rho_0$  is a maximally mixed state. Hence,

$$I_L^T \approx I_L(\rho_1 \otimes \rho_0) = I_L(\rho_1) + I_L(\rho_0) = I_L(\rho_1) \quad (6.6)$$

implies

$$\langle I_L^T \rangle \sim \langle I_{L_c}^T \rangle \sim 2(\ln 2)(\ln L_c)/3 \sim 4(\ln 2)[\ln \ln(1/T)]/3, \quad \langle I_L^T \rangle \sim \langle I_L^{T=0} \rangle \sim 2(\ln 2)(\ln L)/3 \quad (6.7)$$

for  $L \gg L_c$  and  $L \ll L_c$ , respectively, or compactly

$$\langle I_L^T \rangle \sim 2(\ln 2)[\ln \min\{L, \ln^2(1/T)\}]/3, \quad (6.8)$$

which is verified numerically in Fig. 6.2.

Any entanglement measure (for mixed states) satisfies the following: (a) It does not increase under local operations and classical communication (LOCC); (b) it reduces to entanglement entropy for maximally entangled states; and (c) other postulates irrelevant to us. See Refs. [122, 67] for details on the axiomatic approach to entanglement measures. Since the states  $\rho_1$  and  $\rho_1 \otimes \rho_0$  can be transformed to each other by LOCC,

$$E_L^T := E_L(e^{-H/T}) \approx E_L(\rho_1 \otimes \rho_0) = E_L(\rho_1) = S_L(\rho_1) = I_L(\rho_1)/2 \approx I_L^T/2 \Rightarrow \langle E_L^T \rangle \sim \langle I_L^T \rangle/2 \quad (6.9)$$

for any entanglement measure  $E$  (including, but not limited to, entanglement cost, distillable entanglement, entanglement of formation, relative entropy of entanglement, squashed entanglement, and logarithmic negativity). Note that logarithmic negativity, while it does not reduce to entanglement entropy for all pure states, does reduce to entanglement entropy for maximally entangled states and hence satisfies the postulate (b) above. We do not expect any of the aforementioned entanglement measures can be computed efficiently even in free-fermion systems.

## 6.5 Random quantum Ising chain and beyond

We now study the random quantum Ising chain [47, 45, 82]. The Hamiltonian is

$$H = \sum_i J_i \sigma_x^i \sigma_x^{i+1} + h_i \sigma_z^i, \quad (6.10)$$

where  $J_i$ 's are i.i.d. and  $h_i$ 's are i.i.d. random variables. The eigenvalues of  $H$  are generically non-degenerate. Let  $\delta = (\overline{\ln|h|} - \overline{\ln|J|})/(\text{var} \ln|h| + \text{var} \ln|J|)$ . At  $\delta = 0$ , the system is critical, and RSRG implies [129]

$$\langle S_L^{T=0} \rangle \sim (\ln 2)(\ln L)/6. \quad (6.11)$$

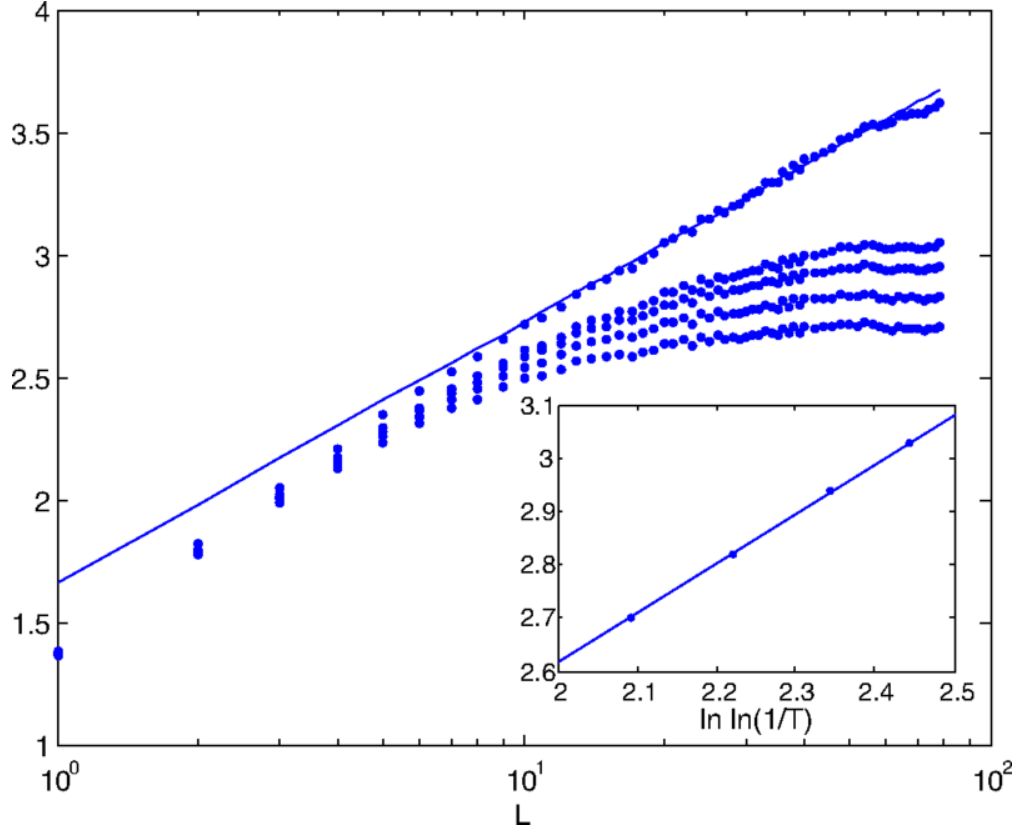


Figure 6.2: (Color online) Scaling of  $\langle I_L^T \rangle$  in random  $XX$  chain. The dots (from top to bottom) are data (averaged over 2500 samples) for  $T = 0, 10^{-5}, 3 \times 10^{-5}, 10^{-4}$ , and  $3 \times 10^{-4}$  in chains of 200 spins. The line is a fit based on (6.7):  $2(\ln 2)(\ln L)/3 + 1.66$ .  $\langle I_L^T \rangle$  behaves as if  $T = 0$  for  $L \ll L_c$  and saturates for  $L \gg L_c$ . Inset: Saturation value  $\langle I_{L \gg L_c}^T \rangle$  vs temperature. The line is a fit based on (6.7):  $4(\ln 2)[\ln \ln(1/T)]/3 + 0.77$ .

Otherwise ( $\delta \neq 0$ ) we expect an area law for  $\langle S_L^{T=0} \rangle$ . Let  $\xi \sim 1/\delta^2$  be the characteristic length scale within and beyond which the system appears critical and noncritical, respectively [45]. The saturation value is  $\langle S_{L \gg \xi}^{T=0} \rangle \sim (\ln 2)(\ln \xi)/6 \sim (\ln 2)(\ln |1/\delta|)/3$  for  $|\delta| \ll 1$ . Straightforward perturbative calculations show that fortunately the difference between effective interactions induced in RSRG and RSRG-X is only in sign [117]. Hence the flow equation and the fixed point solution for the distributions of  $|J_i|, |h_i|$ 's in RSRG-X are identical to those in RSRG. Moreover, the amount of entanglement generated in RSRG-X is the same as that generated in RSRG. Therefore  $\langle S_L^{\forall T} \rangle \sim \langle S_L^{T=0} \rangle$ , which is verified numerically in Fig. 6.3.

Consider the weakly interacting model  $H' = H + \sum_i J'_i \sigma_z^i \sigma_z^{i+1}$ , where  $H$  is the random quantum Ising Hamiltonian (6.10), and  $J'_i$ 's ( $\ll J_i, h_i$ 's) are i.i.d. random variables. This model is studied using RSRG-X in Ref. [117]: There is strong numerical evidence for a temperature-tuned dynamical quantum phase transition. After developing intuitions about

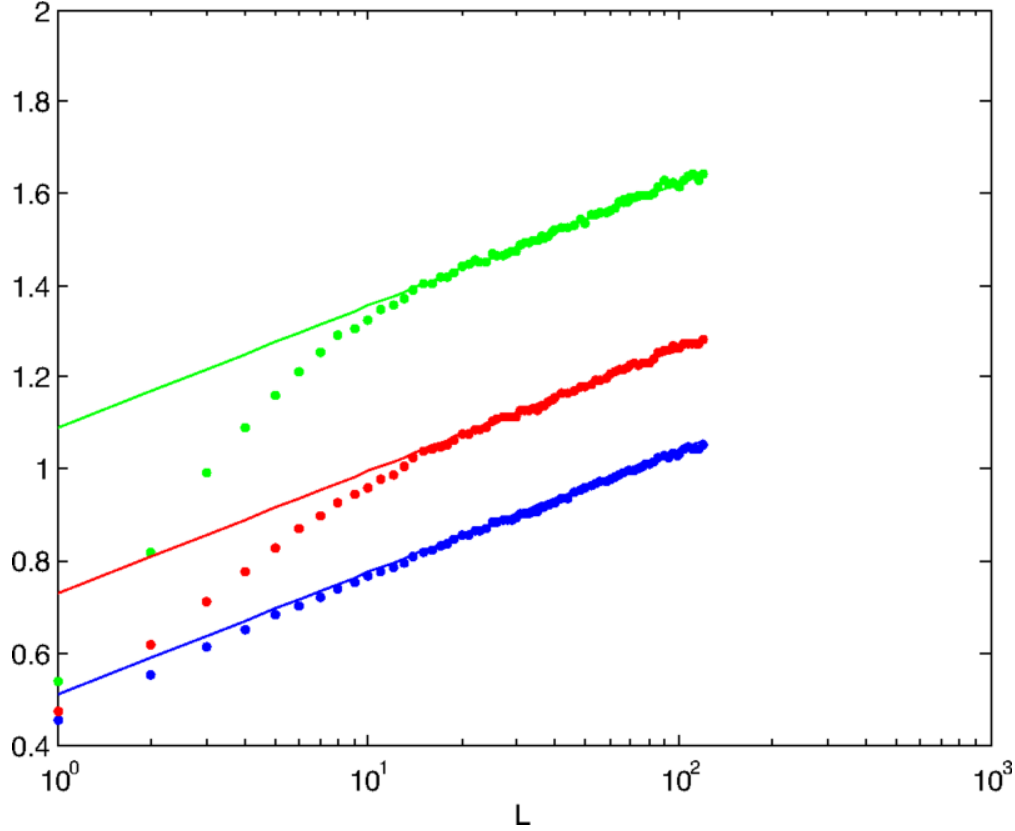


Figure 6.3: (Color online) Scaling of  $\langle S_L^T \rangle$  in critical random quantum Ising chain ( $\delta = 0$ ). Here  $J_i, h_i$ 's are i.i.d. uniform random variables on the interval  $[0, 1]$ . The blue, red, and green dots are data (averaged over 2500 samples) for  $T = 0, 0.2$ , and  $\infty$ , respectively, in chains of 400 spins. The lines are fits based on (6.11):  $(\ln 2)(\ln L)/6 + 0.51$  (blue),  $(\ln 2)(\ln L)/6 + 0.73$  (red), and  $(\ln 2)(\ln L)/6 + 1.09$  (green).

this transition, the scaling of entanglement will be clear.

Irrelevant perturbations do not change the universality class of phase transitions, but they modify the strength of relevant terms. In RSRG-X, the  $J'$  perturbations are irrelevant [117]. Let  $\delta_r(\delta, T, J')$  be the “renormalized  $\delta$ ,” which is a function of  $T$  because the implementation of RSRG-X is temperature dependent. The critical temperature  $T_c$  is given by  $\delta_r(\delta, T_c, J') = 0$ . Therefore,

$$\langle S_L^{T=T_c} \rangle \sim (\ln 2)(\ln L)/6. \quad (6.12)$$

We expect an area law for  $\langle S_L^{T \neq T_c} \rangle$ , and the saturation value is  $\sim (\ln 2)[\ln |1/(T - T_c)|]/3$  for  $|T - T_c| \ll 1$  (and finite  $T_c$ ).

## Chapter 7

# Quantum circuit complexity of one-dimensional topological phases

Topological quantum states cannot be created from product states with local quantum circuits of constant depth and are in this sense more entangled than topologically trivial states, but how entangled are they? Here we quantify the entanglement in 1D topological states by showing that local quantum circuits of linear depth are necessary to generate them from product states. We establish this linear lower bound for both bosonic and fermionic one-dimensional topological phases and use symmetric circuits for phases with symmetry. We also show that the linear lower bound can be saturated by explicitly constructing circuits generating these topological states. The same results hold for local quantum circuits connecting topological states in different phases.

### 7.1 Introduction

Many-body entanglement is essential to the existence of topological order in strongly correlated systems. While ground states in topologically trivial phases can take a simple product form, ground states in topological phases are always entangled. Of course, ground states in topologically trivial phases can be entangled, too. It is then natural to ask what is the essential difference between the entanglement patterns that give rise to topologically trivial and nontrivial states.

Besides topological entanglement entropy [92, 98] and the entanglement spectrum [99], which partially capture the topological properties of the system, quantum circuits provide a powerful tool for characterizing the entanglement patterns of topological states. Intuitively, one would expect that states with more complicated entanglement patterns require larger circuits to generate from product states. Also, small circuits would suffice to connect ground states in the same phase as their entanglement patterns are similar, while large circuits are necessary to map states from one phase to another.

Indeed, in gapped quantum many-body systems it has been shown that two ground states

are in the same topological phase if and only if they can be mapped to each other with a local quantum circuit of constant depth, i.e., a constant (in the system size) number of layers of non-overlapping local unitaries [31]. States with nontrivial intrinsic topological order are thus said to be long-range entangled in the sense that they cannot be created from product states with circuits of constant depth. Circuits of constant depth can generate SPT states from product states but only if the symmetry is broken. If only symmetric unitaries are allowed, the circuit depth has to grow with the system size.

Therefore, topological states are in this sense more entangled than topologically trivial states, but how entangled are they? In particular, we ask, what is the quantum circuit complexity of generating topological states from product states, i.e., how does the circuit depth scale with the system size? In two and higher dimensions, it has been shown that circuits of linear (in the diameter of the system) depth are necessary to generate states with topological degeneracy [22]. One might expect that topological states without topological degeneracy are less entangled and can be created with circuits of sub-linear depth. However, we show that this is not the case, at least in 1D.

We demonstrate that, *to generate 1D gapped (symmetry protected) topological states from product states, the depth of the (symmetric) local quantum circuits has to grow linearly with the system size.* The Majorana chain [90] provides an example of a topological state without topological degeneracy, and we show that local fermionic circuits of linear depth are necessary for its creation. For all 1D SPT states, we show that linear depth is required as long as the symmetry is preserved. In particular, we prove that the nonlocal (string) order parameters [55, 125] distinguishing different SPT phases remain invariant under symmetric circuits of sub-linear depth. Furthermore, we explicitly construct circuits of linear depth that generate 1D topological states. These results suggest the dichotomous picture that ground states of gapped local Hamiltonians are connected by local quantum circuits of either constant or linear depth, depending on whether they are in the same phase or not.

The chapter is organized as follows. Section 7.2 reviews the basic notion of gapped quantum phases and how 1D topological phases are classified with local quantum circuits. Then we study the quantum circuit complexity of prototypical examples of 1D topological phases: the Majorana chain in fermionic systems (Sec. 7.3) and the Haldane chain with  $Z_2 \times Z_2$  on-site symmetry in bosonic (spin) systems (Sec. 7.4). We explicitly construct circuits of linear depth that generate these topological states from product states and show that linear depth is a lower bound. For the Majorana chain, the circuit is composed of fermionic local unitaries; for the Haldane chain with symmetry, the circuit is composed of symmetric local unitaries. Appendix 7.8 establishes the same results for all 1D topological phases in a similar but more complicated way. Section 7.5 concludes with the implications of our results.

## 7.2 Preliminaries

We first review the basic notions of gapped quantum phases and local quantum circuits.

**Definition 16** (gapped quantum phase). Two gapped local Hamiltonians  $H_0$  and  $H_1$  are in the same phase if and only if there exists a smooth path of gapped local Hamiltonians  $H(t)$  with  $0 \leq t \leq 1$  such that  $H(0) = H_0$  and  $H(1) = H_1$ . Correspondingly, their ground states are said to be in the same phase.

Indeed, gapped phases can be defined purely in terms of the ground states, without referring to their Hamiltonians at all. To do this, we need local quantum circuits.

**Definition 17** (local quantum circuit). A local quantum circuit  $C$  of depth  $m$  has a layered structure of local unitary quantum gates,

$$C = \prod_{i_m} C_{i_m}^{(m)} \prod_{i_{m-1}} C_{i_{m-1}}^{(m-1)} \cdots \prod_{i_1} C_{i_1}^{(1)}, \quad (7.1)$$

where in each layer  $1 \leq k \leq m$  the supports of the local unitaries  $C_{i_k}^{(k)}$ 's are pairwise non-intersecting.

**Theorem 6** (informal statement). *Gapped ground states in the same phase are connected by local quantum circuits of constant depth (up to some reasonably small error).*

*Remark.* See Theorem 8 for the formal statement of Theorem 6.

Theorem 6 was discussed in Ref. [31] using quasi-adiabatic continuation [63, 26] and the Lieb-Robinson bound [100, 105, 64]. Gapped phases can also be defined in the presence of symmetry.

**Definition 18** (SPT phase). In the absence of symmetry breaking, two symmetric gapped local Hamiltonians  $H_0$  and  $H_1$  are in the same SPT phase if and only if there exists a smooth path of symmetric gapped local Hamiltonians  $H(t)$  with  $0 \leq t \leq 1$  such that  $H(0) = H_0$  and  $H(1) = H_1$ .

SPT phases can also be defined purely in terms of the symmetric ground states.

**Definition 19** (symmetric local quantum circuit). A local quantum circuit  $C$  is symmetric if each quantum gate  $C_{i_k}^{(k)}$  is symmetric.

**Corollary 3** (informal statement). *Symmetric gapped ground states in the same SPT phase are connected by symmetric local quantum circuits of constant depth (up to some reasonably small error).*

*Remark.* See Corollary 4 for the formal statement of Corollary 3.

Based on Theorem 6 and Corollary 3, 1D gapped phases have been classified [126, 29, 30, 144, 44, 136]. It was found that there is no topological phase in 1D bosonic (spin) systems without symmetry. In 1D fermionic systems without extra symmetry (beyond fermion parity which is always preserved), there is one and only one topological phase: the Majorana

chain with Majorana edge modes [90]. In 1D systems with (extra) symmetry, there can be SPT phases with degenerate edge states carrying projective representations of the symmetry group. See Appendix 7.7 for the classification of 1D SPT phases.

Since (symmetry protected) topological states cannot be mapped to topologically trivial states (including product states) with (symmetric) local quantum circuits of constant depth, we ask, what circuit depth is necessary to do this mapping? We show that linear depth is necessary by proving the invariance of the nonlocal (string) order parameters [14, 55, 125] distinguishing different (symmetry protected) topological phases under (symmetric) circuits of sub-linear depth.

**Theorem 7.** *Suppose  $|\psi\rangle$  and  $C|\psi\rangle$  are two gapped ground states in 1D systems (with symmetry), where  $C$  is a (symmetric) local quantum circuit of sub-linear depth. Then  $|\psi\rangle$  and  $C|\psi\rangle$  are in the same (symmetry protected) topological phase.*

### 7.3 Majorana chain

In the absence of (extra) symmetry (beyond fermion parity), the Majorana chain with Majorana edge modes [90] is the only 1D topological order. We now study the Majorana chain by considering the fermionic model

$$H = \sum_{j=1}^{N-1} (a_j - a_j^\dagger) (a_{j+1} + a_{j+1}^\dagger) + \mu \sum_{j=1}^N (2a_j^\dagger a_j - 1) - (a_N - a_N^\dagger) (a_1 + a_1^\dagger) \quad (7.2)$$

with anti-periodic boundary conditions in the symmetry sector of even fermion parity, where  $a_j$  and  $a_j^\dagger$  are the fermion annihilation and creation operators at the site  $j$ . This model is in the topologically trivial and nontrivial phases for  $\mu > 1$  and  $0 \leq \mu < 1$ , respectively. We show that two ground states in different phases can be connected by a local fermionic circuit of linear depth and that linear depth is a lower bound.

**Proposition 3.** *Suppose  $|\psi_0\rangle$  and  $|\psi_1\rangle$  are two gapped ground states in the topologically trivial and nontrivial phases in 1D fermionic systems, respectively. Given an arbitrarily small constant  $\epsilon$ , there exist  $|\psi'_0\rangle, |\psi'_1\rangle$  and a local fermionic circuit  $C$  of linear depth such that  $|\psi'_1\rangle = C|\psi'_0\rangle$  and*

$$|\langle \psi_k | P | \psi_k \rangle - \langle \psi'_k | P | \psi'_k \rangle| \leq \epsilon \quad (k = 0, 1) \quad (7.3)$$

for any local operator  $P$  with bounded norm.

*Proof.* Define two Majorana operators at each site:

$$c_{2j-1} = a_j + a_j^\dagger, \quad c_{2j} = (a_j - a_j^\dagger) / i. \quad (7.4)$$

At  $\mu = +\infty$ ,  $H = i\mu \sum_{j=1}^N c_{2j-1} c_{2j}$  is in the trivial phase, and its ground state  $|\phi_0\rangle$  is the tensor product of the vacuum states of the modes  $a_j = (c_{2j-1} + i c_{2j}) / 2$ . At  $\mu = 0$ ,



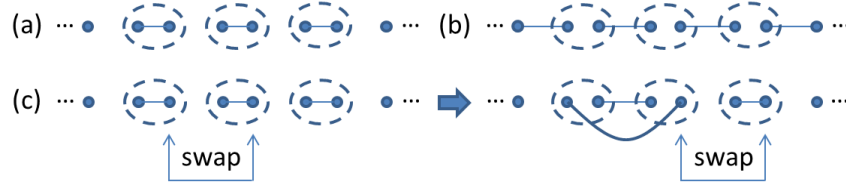


Figure 7.1: (Color online) The renormalization group (RG) fixed-point states [148, 29] in the (a) trivial and (b) nontrivial fermionic (Majorana chain) or SPT (e.g., Haldane chain) phases. For states in fermionic phases, each dot represents a Majorana mode and connected pairs form fermionic modes which are vacant or occupied. For states in SPT phases, each dot carries a projective representation of the symmetry group and connected pairs form symmetric singlets. (c) The states in (a) and (b) can be exactly mapped to each other with a linear-depth 2-local quantum circuit composed of SWAP gates.

$H = i \sum_{j=1}^{N-1} c_{2j} c_{2j+1} - i c_{2N} c_1$  is in the nontrivial phase, and its ground state  $|\phi_1\rangle$  is the tensor product of the vacuum (or occupied) states of the fermionic modes  $b_j = (c_{2j} + i c_{2j+1})/2$ . Figure 7.1(a) and (b) illustrate the structures of  $|\phi_0\rangle$  and  $|\phi_1\rangle$ , which are the RG fixed-point states in the topologically trivial and nontrivial phases, respectively.

As shown in Fig. 7.1(c),  $|\phi_0\rangle$  and  $|\phi_1\rangle$  can be exactly mapped to each other with a 2-local fermionic circuit

$$C_\phi = \prod_{j=N-1}^1 C^{(j)}, \quad C^{(j)} = \frac{c_{2j+2} c_{2j+1} + c_{2j+1} c_{2j}}{\sqrt{2}} \quad (7.5)$$

of depth  $N - 1$ , where the local unitary  $C^{(j)}$  swaps  $c_{2j}$  and  $c_{2j+2}$ . As  $|\psi_k\rangle$  and  $|\phi_k\rangle$  are in the same phase, there exists a local fermionic circuit  $C_k$  of constant depth (Appendix 7.6) such that  $|\langle \psi_k | P | \psi_k \rangle - \langle \psi'_k | P | \psi'_k \rangle| \leq \epsilon$  for any local operator  $P$  with bounded norm, where  $|\psi'_k\rangle = C_k |\phi_k\rangle$ . Finally,  $C = C_1 C_\phi C_0^\dagger$  is the circuit of linear depth that connects  $|\psi_0\rangle$  and  $|\psi_1\rangle$ .  $\square$

**Proposition 4.** *Suppose  $|\psi\rangle$  and  $C|\psi\rangle$  are two gapped ground states in 1D fermionic systems, where  $C$  is a local fermionic circuit of sub-linear depth. Then  $|\psi\rangle$  and  $C|\psi\rangle$  are in the same topological phase.*

*Proof.* The string order parameter

$$\lim_{N \rightarrow +\infty} \left\langle \left( a_{\frac{N}{3}}^\dagger + a_{\frac{N}{3}} \right) \prod_{j=\frac{N}{3}}^{\frac{2N}{3}-1} e^{i\pi a_j^\dagger a_j} \left( a_{\frac{2N}{3}}^\dagger + a_{\frac{2N}{3}} \right) \right\rangle \quad (7.6)$$

is zero in the topologically trivial phase and nonzero in the topologically nontrivial phase [14]. We show that its value cannot change between these two cases under local fermionic circuits of sub-linear depth.

This is easiest to see by applying the Jordan-Wigner transformation

$$a_k = \sigma_k^- \prod_{j=1}^{k-1} (-\sigma_j^z), \quad a_k^\dagger = \sigma_k^+ \prod_{j=1}^{k-1} (-\sigma_j^z), \quad (7.7)$$

where  $\sigma_k^-$  and  $\sigma_k^+$  are the spin-1/2 lowering and raising operators at the site  $k$ . The fermionic model (7.2) is mapped to the transverse field Ising model with periodic boundary conditions:

$$H = - \sum_{j=1}^{N-1} \sigma_j^x \sigma_{j+1}^x - \sigma_N^x \sigma_1^x + \mu \sum_{j=1}^N \sigma_j^z, \quad (7.8)$$

and the string order parameter (7.6) is mapped to  $\lim_{N \rightarrow +\infty} \langle \psi_s | \sigma_{N/3}^x \sigma_{2N/3}^x | \psi_s \rangle$ , where  $|\psi_s\rangle$  is the spin ground state. This spin model is in the disordered phase for  $\mu > 1$  with vanishing correlations at large distances, e.g.,  $\lim_{N \rightarrow +\infty} \langle \psi_s | \sigma_{N/3}^x \sigma_{2N/3}^x | \psi_s \rangle = 0$ , and it is in the ordered phase for  $0 \leq \mu < 1$  with long-range correlations:  $\lim_{N \rightarrow +\infty} \langle \psi_s | \sigma_{N/3}^x \sigma_{2N/3}^x | \psi_s \rangle > 0$ . As any local unitary in 1D fermionic systems remains local after the nonlocal Jordan-Wigner transformation [in the case where the local unitary in 1D fermionic systems crosses the boundary, there is a trivial factor  $\prod_{j=1}^N (-\sigma_j^z) = 1$  as the fermion parity is even], a local fermionic circuit  $C$  of sub-linear depth is mapped to a local spin circuit  $C_s$  of sub-linear depth. The Lieb-Robinson bound states that correlations can only propagate at a finite speed in quantum many-body systems with local interactions [100, 105, 64]. As a consequence, local quantum circuits of sub-linear depth cannot generate long-range order [22], i.e.,  $\lim_{N \rightarrow +\infty} \langle \psi_s | C_s^\dagger \sigma_{N/3}^x \sigma_{2N/3}^x C_s | \psi_s \rangle = 0$  for any state  $|\psi_s\rangle$  with vanishing correlations at large distances. Therefore, the string order parameter (7.6) is either both zero or both nonzero for the fermionic states  $|\psi\rangle$  and  $C|\psi\rangle$ .  $\square$

## 7.4 Haldane chain

We switch to 1D spin systems. In the absence of symmetry, all 1D gapped spin systems are in the same phase. In the presence of symmetry, however, there can be SPT phases with degenerate edge states carrying projective representations of the symmetry group [126, 29, 30, 136]. See Appendix 7.7 for the classification of 1D SPT phases, which includes a brief review of projective representations. SPT states are short-range entangled in the sense that they can be created from product states with local quantum circuits of constant depth by breaking the symmetry. If the symmetry is preserved, we show that two ground states in different SPT phases can be connected by a local quantum circuit of linear depth and that linear depth is a lower bound.

We now study the Haldane chain with  $Z_2 \times Z_2$  on-site symmetry as a prototypical example, where we use periodic boundary conditions so that the ground state is unique and symmetric. The proof for general 1D SPT phases is similar but more complicated (Appendix 7.8). With  $Z_2 \times Z_2$  symmetry, there are two phases [126, 124]: the trivial phase and the Haldane (nontrivial SPT) phase [56, 57].

**Proposition 5.** *Suppose  $|\psi_0\rangle$  and  $|\psi_1\rangle$  are two  $Z_2 \times Z_2$  symmetric gapped ground states in the trivial and the Haldane phases, respectively. Given an arbitrarily small constant  $\epsilon$ , there exist  $|\psi'_0\rangle, |\psi'_1\rangle$  and a symmetric local quantum circuit  $C$  of linear depth such that  $|\psi'_1\rangle = C|\psi'_0\rangle$  and*

$$|\langle \psi_k | P | \psi_k \rangle - \langle \psi'_k | P | \psi'_k \rangle| \leq \epsilon \quad (k = 0, 1) \quad (7.9)$$

for any local operator  $P$  with bounded norm.

*Proof.* The proof proceeds analogously to that of Proposition 3. Figure 7.1(a) and (b) illustrate the structures of the RG fixed-point states  $|\phi_0\rangle$  and  $|\phi_1\rangle$  in the trivial and the Haldane phases, respectively, where each dot now represents a spin-1/2 degree of freedom transforming projectively under  $\pi$  rotations about the  $x, y, z$  axes. It is apparent that the edge state of  $|\phi_1\rangle$  in the Haldane phase is twofold degenerate and transforms projectively while that of  $|\phi_0\rangle$  in the trivial phase is trivial.

As shown in Fig. 7.1(c),  $|\phi_0\rangle$  and  $|\phi_1\rangle$  can be exactly mapped to each other by applying  $(N-1)$  2-local SWAP gates sequentially. These SWAP gates rearrange the singlets, are  $Z_2 \times Z_2$  symmetric and form a symmetric 2-local quantum circuit  $C_\phi$  of depth  $N-1$ . As  $|\psi_k\rangle$  and  $|\phi_k\rangle$  are in the same SPT phase, there exists a symmetric local quantum circuit  $C_k$  of constant depth (Appendix 7.6) such that  $|\langle \psi_k | P | \psi_k \rangle - \langle \psi'_k | P | \psi'_k \rangle| \leq \epsilon$  for any local operator  $P$  with bounded norm, where  $|\psi'_k\rangle = C_k|\phi_k\rangle$ . Finally,  $C = C_1 C_\phi C_0^\dagger$  is the symmetric circuit of linear depth that connects  $|\psi_0\rangle$  and  $|\psi_1\rangle$ .  $\square$

**Proposition 6.** *Suppose  $|\psi\rangle$  and  $C|\psi\rangle$  are two symmetric gapped ground states in 1D spin systems with  $Z_2 \times Z_2$  on-site symmetry represented by  $\{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$ , where  $C$  is a symmetric local quantum circuit of sub-linear depth. Then  $|\psi\rangle$  and  $C|\psi\rangle$  are in the same SPT phase.*

*Proof.* We make use of the string (nonlocal) order parameters [55, 125] distinguishing different SPT phases. For the Haldane chain, the string order operator is [108, 88, 87]

$$Q = S_{N/3}^y \prod_{j=N/3+1}^{2N/3-1} e^{i\pi S_j^y} S_{2N/3}^y, \quad (7.10)$$

where  $\vec{S}_j = (S_j^x, S_j^y, S_j^z)$  is the spin-1 operator at the site  $j$ . The string order parameter  $\lim_{N \rightarrow +\infty} \langle Q \rangle$  is zero in the trivial phase and nonzero in the Haldane phase. We show that its value cannot change between these two cases under  $Z_2 \times Z_2$  symmetric local quantum circuits of sub-linear depth.

Assume without loss of generality that  $C$  is a symmetric 2-local quantum circuit of depth  $m \leq N/9$ . Figure 7.2 shows the expectation value  $\langle \psi | C^\dagger Q C | \psi \rangle$ . As each gate in the circuit  $C$  is unitary and symmetric, the white gates cancel out. Then we merge the gray gates inside the causal cones (dotted lines) of the left and right end operators  $S^y$  (small open red squares) into  $C_l$  and  $C_r$ , respectively. As  $C$  is of sub-linear depth,  $C_l$  and  $C_r$  are non-overlapping.

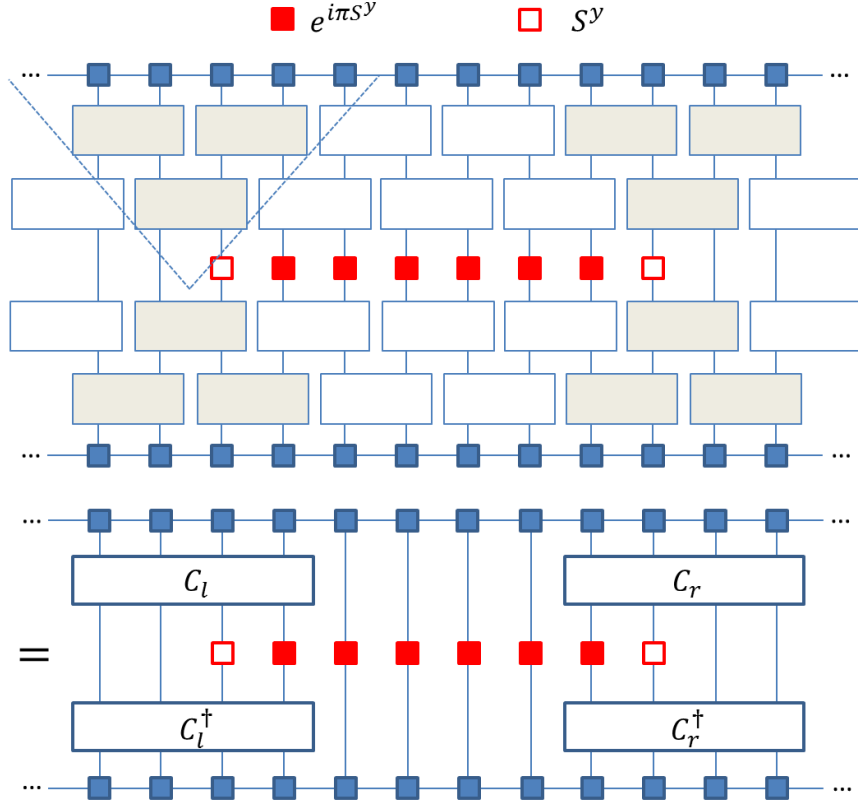


Figure 7.2: (Color online) The expectation value  $\langle \psi | C^\dagger Q C | \psi \rangle$ . The horizontal lines attached with small blue squares represent  $\langle \psi |$  (bra) or  $|\psi\rangle$  (ket), and the short rectangles are the 2-local unitaries in  $C$ . The (white) unitaries outside the causal cones (dotted lines) of  $S^y$  (small open red squares) can be removed, as they are symmetric. Then we merge the (gray) symmetric local quantum gates inside each casual cone into one symmetric quantum gate (long rectangle) of sub-linear support.

Hence  $Q' = C^\dagger Q C$  remains a string (order) operator. Specifically, the string becomes shorter but is still of the form  $\prod_j e^{i\pi S_j^y}$ . The left and right end operators are changed to

$$Q_l = C_l^\dagger S_{N/3}^y \prod_{j=N/3+1}^{N/3+m} e^{i\pi S_j^y} C_l, \quad Q_r = C_r^\dagger \prod_{j=2N/3-m}^{2N/3-1} e^{i\pi S_j^y} S_{2N/3}^y C_r, \quad (7.11)$$

respectively. As  $C_l$  is symmetric,  $Q_l$  transforms in the same way under the symmetry as  $S^y$ , e.g.,

$$\prod_j e^{-i\pi S_j^z} Q_l \prod_j e^{i\pi S_j^z} = -Q_l. \quad (7.12)$$

Appendix 7.8 shows that  $\lim_{N \rightarrow +\infty} \langle \psi | Q' | \psi \rangle = 0$  if and only if  $\lim_{N \rightarrow +\infty} \langle \psi | Q | \psi \rangle = 0$ . Therefore, the string order operator (7.10) has either both zero or both nonzero expectation values

for  $|\psi\rangle$  and  $C|\psi\rangle$ .  $\square$

Nonlocal (string) order parameters have been systematically constructed for general 1D SPT phases [55, 125]. Appendix 7.8 extends our proof to all these cases accordingly.

## 7.5 Conclusion

We have quantified the many-body entanglement in 1D (symmetry protected) topological states with (symmetric) local quantum circuits. In particular, we have shown that circuits of linear depth are necessary to generate 1D topological states from product states. We have also explicitly constructed circuits of linear depth that generate 1D topological states. These results are useful not only conceptually but also operationally as a guide to preparing topological states in experiments.

Although our proof is in 1D, we expect similar results in two and higher dimensions. Indeed, it has been shown that local quantum circuits of linear (in the diameter of the system) depth are necessary to generate states with topological degeneracy [22]. We conjecture that this is also true for topological states without topological degeneracy, e.g., the integer quantum Hall states, the  $p$ -wave superconductors, and the  $E_8$  states. See Ref. [54] for recent progress in this direction.

More generally, we can ask, what is the quantum circuit complexity of generating ground states in gapless phases or at phase transitions? We expect that quantum circuits also characterize the entanglement patterns that give rise to the physical properties in gapless or critical systems.

**Acknowledgments.** We would like to thank Isaac H. Kim, Spyridon Michalakis, Joel E. Moore, John Preskill, Frank Pollmann, and Ashvin Vishwanath for helpful discussions. In particular, I.H.K. pointed out that a variant of Proposition 4 can be proved using his entropic topological invariant [89].

## 7.6 Appendix: States in the same phase

We give a rigorous formulation of the statement [31] that gapped ground states in the same phase are connected by local quantum circuits of constant depth.

**Lemma 45.** *Suppose  $H_0(t)$  and  $H_1(t)$  are two time-dependent Hamiltonians with  $\|H_0(t) - H_1(t)\| \leq \delta$ . Then the (unitary) time-evolution operators*

$$U_k(t) = \mathcal{T} e^{-i \int_0^t H_k(\tau) d\tau} \quad (k = 0, 1) \tag{7.13}$$

*satisfy  $\|U_0(t) - U_1(t)\| \leq \delta t$ , where  $\mathcal{T}$  is the time-ordering operator.*

*Proof.* Let

$$U_I(t) = \mathcal{T} e^{-i \int_0^t U_0^\dagger(\tau) [H_1(\tau) - H_0(\tau)] U_0(\tau) d\tau} \quad (7.14)$$

be the (unitary) time-evolution operator in the interaction picture. Indeed, it is straightforward to verify  $U_1(t) = U_0(t)U_I(t)$  by differentiating with respect to  $t$ . Then,

$$\begin{aligned} \|U_I'(t)\| &= \left\| U_0^\dagger(t)(H_1(t) - H_0(t))U_0(t)U_I(t) \right\| = \|H_1(t) - H_0(t)\| \leq \delta \\ \Rightarrow \|U_0(t) - U_1(t)\| &= \|U_0(t)U_I(0) - U_0(t)U_I(t)\| = \|U_I(0) - U_I(t)\| \leq \delta t. \end{aligned} \quad (7.15)$$

□

**Lemma 46.** *Suppose  $H(t) = \sum_{j=1}^{N-1} h^{(j)}(t)$  is a time-dependent 1D 2-local Hamiltonians with open boundary conditions, where  $h^{(j)}$  acts on the spins  $j$  and  $j + 1$  (nearest-neighbor interaction). Define  $H_*(t) = \sum_{j=1}^{l-1} h^{(j)}(t)$  for  $l \leq N$ . Let  $U(t)$  and  $U_*(t)$  be the (unitary) time-evolution operators for  $H(t)$  and  $H_*(t)$ , respectively. Then,*

$$\|U^\dagger(1)PU(1) - U_*^\dagger(1)PU_*(1)\| = e^{-\Omega(l)} \quad (7.16)$$

for any operator  $P$  acting on the first spin with  $\|P\| \leq 1$ .

Lemma 46 is a variant of the Lieb-Robinson bound [100, 105, 64]. See Ref. [24] in Ref. [112] for a simple direct proof.

**Theorem 8** (formal statement of Theorem 6). *Suppose  $|\psi_0\rangle$  and  $|\psi_1\rangle$  are two gapped ground states in the same phase in any spatial dimension. Given an arbitrarily small constant  $\epsilon = \Theta(1)$ , there exists a local quantum circuit  $C$  of depth  $O(1)$  such that*

$$|\langle \psi_1 | P | \psi_1 \rangle - \langle \psi_0 | C^\dagger P C | \psi_0 \rangle| \leq \epsilon \quad (7.17)$$

for any local operator  $P$  with  $\|P\| \leq 1$ .

*Proof.* By Definition 16, there exists a smooth path of gapped local Hamiltonians  $H_0(t)$  with  $0 \leq t \leq 1$  such that  $|\psi_0\rangle$  and  $|\psi_1\rangle$  are the ground states of  $H_0(0)$  and  $H_0(1)$ , respectively. Quasi-adiabatic continuation [63] defines a smooth time-dependent local Hamiltonian  $H_1(t)$  such that

$$|\langle \psi_1 | P | \psi_1 \rangle - \langle \psi_0 | U_1^\dagger(1) P U_1(1) | \psi_0 \rangle| \leq \epsilon/3 \quad (7.18)$$

for any local operator  $P$  with  $\|P\| \leq 1$ . Assume without loss of generality that  $H_1(t) = \sum_{j=1}^{N-1} h_1^{(j)}(t)$  is a 1D 2-local Hamiltonian with open boundary conditions and that  $P$  is an operator acting on the first spin. We approximate the time-dependent Hamiltonian  $H_1(t)$  by the piecewise time-independent Hamiltonian

$$\sum_{j=1}^{N-1} h_2^{(j)} = H_2(t) := H_1([rt]/r) = \sum_{j=1}^{N-1} h_1^{(j)}([rt]/r) \quad (7.19)$$

with sufficiently large  $r = O(1)$ . Let  $l = O(1)$  be a cutoff and define

$$H_3(t) = \sum_{j=1}^{l-1} h_1^{(j)}(t) + \sum_{j=l}^{N-1} h_2^{(j)}(t). \quad (7.20)$$

Lemma 46 implies

$$\left\| U_1^\dagger(1)PU_1(1) - U_3^\dagger(1)PU_3(1) \right\| \leq \epsilon/6 \quad (7.21)$$

for sufficiently large  $l = O(1)$ . As  $H_1(t)$  is smooth, Lemma 45 implies

$$\begin{aligned} \lim_{r \rightarrow +\infty} \left\| h_1^{(j)}(t) - h_2^{(j)}(t) \right\| = 0 &\Rightarrow \|H_3(t) - H_2(t)\| \leq \sum_{j=1}^{l-1} \left\| h_1^{(j)}(t) - h_2^{(j)}(t) \right\| \leq \epsilon/12 \\ \Rightarrow \|U_3(1) - U_2(1)\| \leq \epsilon/12 &\Rightarrow \left\| U_3^\dagger(1)PU_3(1) - U_2^\dagger(1)PU_2(1) \right\| \leq \epsilon/6 \end{aligned} \quad (7.22)$$

for sufficiently large  $r = O(l/\epsilon) = O(1)$ . Hence,

$$\left\| U_1^\dagger(1)PU_1(1) - U_2^\dagger(1)PU_2(1) \right\| \leq \epsilon/3. \quad (7.23)$$

As  $H_2(t)$  is piecewise time independent, assume without loss of generality that it is time independent. Define

$$H_2 = H^o + H^e, \quad H^o = \sum_{j=1}^{[N/2]} h_2^{(2j-1)}, \quad H^e = \sum_{j=1}^{[(N-1)/2]} h_2^{(2j)} \quad (7.24)$$

such that the first-order Trotter decomposition is given by

$$U_2(1) = \left( e^{-iH^o/s - iH^e/s} \right)^s \approx \left( e^{-iH^o/s} e^{-iH^e/s} \right)^s = \left( \prod_{j=1}^{[N/2]} e^{-ih_2^{(2j-1)}/s} \prod_{j=1}^{[(N-1)/2]} e^{-ih_2^{(2j)}/s} \right)^s =: C, \quad (7.25)$$

where  $C$  is a 2-local quantum circuit of depth  $2s$ . Let  $L = O(1)$  be a cutoff and define

$$H_* = \sum_{j=1}^{L-1} h_2^{(j)} = H_*^o + H_*^e, \quad H_*^o = \sum_{j=1}^{[L/2]} h_2^{(2j-1)}, \quad H_*^e = \sum_{j=1}^{[(L-1)/2]} h_2^{(2j)}. \quad (7.26)$$

Similarly,

$$U_*(1) = \left( e^{-iH_*^o/s - iH_*^e/s} \right)^s \approx \left( e^{-iH_*^o/s} e^{-iH_*^e/s} \right)^s = \left( \prod_{j=1}^{[L/2]} e^{-ih_2^{(2j-1)}/s} \prod_{j=1}^{[(L-1)/2]} e^{-ih_2^{(2j)}/s} \right)^s =: C_*, \quad (7.27)$$

where  $C_*$  is also a 2-local quantum circuit of depth  $2s$ . The standard error analysis of the Trotter decomposition leads to

$$\|H_*\| = O(L) = O(1) \Rightarrow \|U_*(1) - C_*\| \leq \epsilon/18 \Rightarrow \|U_*^\dagger(1)PU_*(1) - C_*^\dagger PC_*\| \leq \epsilon/9 \quad (7.28)$$

for sufficiently large  $s = O(1)$ . We observe that  $C = \mathcal{T}e^{-i \int_0^2 H^C(t) dt}$  is the (unitary) time-evolution operator for the piecewise time-independent Hamiltonian  $H^C(t)$ , where  $H^C(t) = H^o$  if  $[st]$  is odd and  $H^C(t) = H^e$  if  $[st]$  is even. Similarly,  $C_* = \mathcal{T}e^{-i \int_0^2 H_*^C(t) dt}$ , where  $H_*^C(t) = H_*^o$  if  $[st]$  is odd and  $H_*^C(t) = H_*^e$  if  $[st]$  is even. Lemma 46 implies

$$\left\| U_2^\dagger(1)PU_2(1) - U_*^\dagger(1)PU_*(1) \right\| \leq \epsilon/9, \quad \|C^\dagger PC - C_*^\dagger PC_*\| \leq \epsilon/9 \quad (7.29)$$

for sufficiently large  $L = O(1)$ . Hence,

$$\left\| U_2^\dagger(1)PU_2(1) - C^\dagger PC \right\| \leq \epsilon/3. \quad (7.30)$$

Finally,

$$\begin{aligned} & |\langle \psi_1 | P | \psi_1 \rangle - \langle \psi_0 | C^\dagger PC | \psi_0 \rangle| \\ & \leq \left| \langle \psi_1 | P | \psi_1 \rangle - \langle \psi_0 | U_1^\dagger(1)PU_1(1) | \psi_0 \rangle \right| + \left| \langle \psi_0 | U_1^\dagger(1)PU_1(1) | \psi_0 \rangle - \langle \psi_0 | C^\dagger PC | \psi_0 \rangle \right| \\ & \leq \epsilon/3 + \left\| U_1^\dagger(1)PU_1(1) - C^\dagger PC \right\| \\ & \leq \epsilon/3 + \left\| U_1^\dagger(1)PU_1(1) - U_2^\dagger(1)PU_2(1) \right\| + \left\| U_2^\dagger(1)PU_2(1) - C^\dagger PC \right\| \\ & \leq \epsilon/3 + \epsilon/3 + \epsilon/3 = \epsilon. \end{aligned} \quad (7.31)$$

□

A minor modification of the proof of Theorem 8 leads to similar results in fermionic systems and/or in the presence of symmetry.

**Corollary 4** (formal statement of Corollary 3). *Suppose  $|\psi_0\rangle$  and  $|\psi_1\rangle$  are two symmetric gapped ground states in the same SPT phase in any spatial dimension. Given an arbitrarily small constant  $\epsilon = \Theta(1)$ , there exists a symmetric local quantum circuit  $C$  of depth  $O(1)$  such that*

$$|\langle \psi_1 | P | \psi_1 \rangle - \langle \psi_0 | C^\dagger PC | \psi_0 \rangle| \leq \epsilon \quad (7.32)$$

for any local operator  $P$  with  $\|P\| \leq 1$ .

The main result of Ref. [114] is an immediate corollary of Theorem 8.

**Corollary 5** (efficient classical simulation of adiabatic quantum computation with a constant gap in any spatial dimension). *Suppose we are given a smooth path of gapped local Hamiltonians  $H(t)$  with  $0 \leq t \leq 1$ , where the ground state  $|\psi_0\rangle$  of  $H(0)$  is simple in the sense that  $\langle \psi_0 | P | \psi_0 \rangle$  can be efficiently computed classically for any local operator  $P$  with  $\|P\| \leq 1$ . Then  $\langle \psi_1 | P | \psi_1 \rangle$  can be efficiently computed classically up to an arbitrarily small constant additive error, where  $|\psi_1\rangle$  is the ground state of  $H(1)$  encoding the solution of the adiabatic quantum computation.*



## 7.7 Appendix: Symmetry protected topological phase

We review the classification of 1D SPT phases, and begin by recalling two key notions: projective representations and MPS.

### Projective representation

In the context of this chapter, a projective representation is a mapping  $u$  from the symmetry group  $G$  to unitary matrices such that

$$u(g_1)u(g_2) = \omega(g_1, g_2)u(g_1g_2), \quad (7.33)$$

where  $\omega(g_1, g_2)$  (called the factor system of the projective representation) is an  $U(1)$  phase factor, cf.  $u$  is a linear representation of  $G$  if the factor system is trivial, i.e.,  $\omega(g_1, g_2) = 1$  for any  $g_1, g_2 \in G$ . The associativity of  $G$  implies

$$\omega(g_2, g_3)\omega(g_1, g_2g_3) = \omega(g_1, g_2)\omega(g_1g_2, g_3). \quad (7.34)$$

Multiplying  $u$  by  $U(1)$  phase factors  $\beta$  leads to a different projective representation  $u'$  with the factor system  $\omega'$ :

$$u'(g) = \beta(g)u(g) \Rightarrow \omega'(g_1, g_2) = \omega(g_1, g_2)\beta(g_1)\beta(g_2)/\beta(g_1g_2), \quad (7.35)$$

Two projective representations  $u$  and  $u'$  are equivalent if and only if they differ only by prefactors. Correspondingly, their factor systems  $\omega$  and  $\omega'$  are said to be in the same equivalence class  $[\omega]$ . Let  $u_1$  and  $u_2$  be two projective representations with the factor systems  $\omega_1$  and  $\omega_2$  in the equivalence classes  $[\omega_1]$  and  $[\omega_2]$ , respectively. Apparently,  $u_1 \otimes u_2$  is a projective presentation with the factor system  $\omega_1\omega_2$  in the equivalence class  $[\omega_1\omega_2]$ . By defining  $[\omega_1] \cdot [\omega_2] = [\omega_1\omega_2]$ , the equivalence classes of factor systems form an Abelian group [called the second cohomology group  $H^2(G, U(1))$ ], where the identity element is the equivalence class that contains the trivial factor system.

### Matrix product state

Suppose we are working with a chain of  $N$  spins (qudits), and the local dimension of each spin is  $d = \Theta(1)$ . Let  $\{|i_k\rangle\}_{i_k=1}^d$  be the computational basis of the Hilbert space of the spin  $k$ .

**Definition 20** (MPS [118, 41]). Let  $\{D_k\}_{k=0}^n$  with  $D_0 = D_n$  be a sequence of positive integers. As illustrated in Fig. 7.3(a), an MPS  $|\Psi\rangle$  takes the form

$$|\Psi\rangle = \sum_{i_1, i_2, \dots, i_N=1}^d \text{tr} \left( A_{i_1}^{(1)} A_{i_2}^{(2)} \cdots A_{i_N}^{(N)} \right) |i_1 i_2 \cdots i_N\rangle, \quad (7.36)$$

where  $A_{i_k}^{(k)}$  is a matrix of size  $D_{k-1} \times D_k$ . Define  $D = \max\{D_k\}_{k=0}^n$  as the bond dimension of the MPS  $|\Psi\rangle$ .

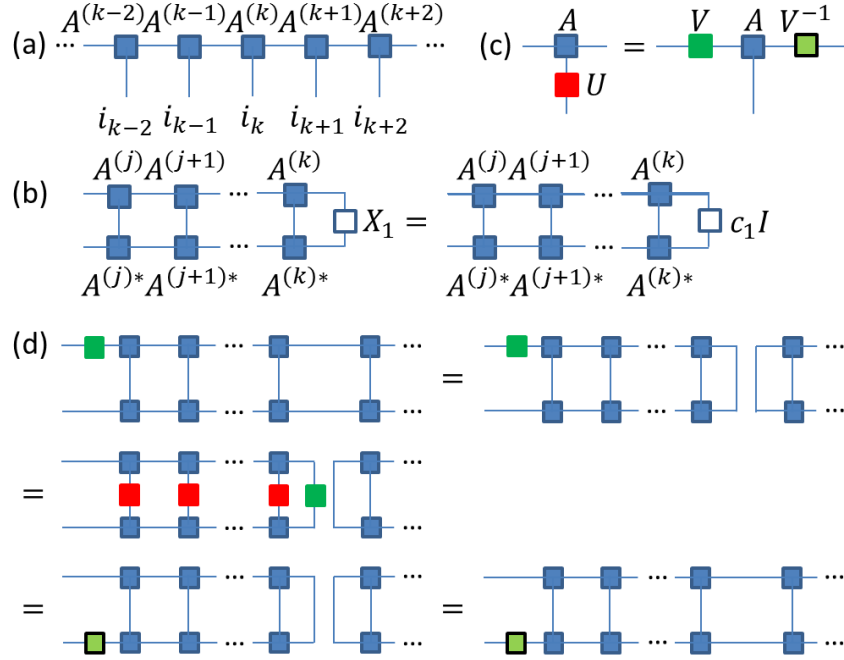


Figure 7.3: (Color online) (a) Graphical representation of MPS (7.36) [133]. Each square represents a tensor  $A^{(k)}$  with two bond indices (horizontal lines) and one physical index (vertical line). The bond indices are contracted sequentially with periodic boundary conditions (not shown). (b) The condition (7.38) for short-range correlated MPS. The graphical equation is approximate up to error  $e^{-\Omega(k-j)}$ , which can be neglected in the thermodynamic limit  $N \rightarrow +\infty$  if  $k - j = \Theta(N)$ . (c) Graphical representation of (7.39). The site labels are not shown. (d) is a consequence of (b) and (c). Note that a prefactor of the second, third, and fourth tensor networks is not shown.

The ground states of 1D gapped Hamiltonians can be represented as MPSs of small bond dimension [59, 10, 70]. The ground states of gapped local Hamiltonians are short-range correlated in the sense that all connected correlation functions decay exponentially with distance [60, 105, 64].

For each  $k$ , define two linear maps

$$\mathcal{E}_k(X) = \sum_{i_k=1}^d A_{i_k}^{(k)} X A_{i_k}^{(k)\dagger}, \quad \mathcal{E}_k^*(X) = \sum_{i_k=1}^d A_{i_k}^{(k)\dagger} X A_{i_k}^{(k)}. \quad (7.37)$$

Any MPS can be transformed into the so-called canonical form [118] such that  $\mathcal{E}_k(I) = I$  and  $\mathcal{E}_k^*(M_{k-1}) = M_k$ , where  $I$  is an identity matrix, and  $M_k$  is a positive diagonal matrix. A canonical MPS is short-range correlated if for any  $X_1, X_2$  with  $\|X_1\|, \|X_2\| \leq 1$  there exist coefficients  $c_1, c_2$  such that

$$\|\mathcal{E}_j \mathcal{E}_{j+1} \cdots \mathcal{E}_k (X_1 - c_1 I)\| = e^{-\Omega(k-j)}, \quad \|\mathcal{E}_k^* \mathcal{E}_{k-1}^* \cdots \mathcal{E}_j^* (X_2 - c_2 M_{j-1})\| = e^{-\Omega(k-j)} \quad (7.38)$$

at large  $k - j$ , i.e.,  $X_1$  can be replaced by  $c_1 I$  up to error  $e^{-\Omega(k-j)}$ , as illustrated in Figure 7.3(b). Hence  $X_1$  (and  $X_2$ ) can be replaced by any matrix up to a multiplicative prefactor and an exponentially small error. When  $A_{i_k}^{(k)}$ 's are site independent (and the MPS  $|\Psi\rangle$  is translationally invariant), (7.38) is equivalent to the condition [41, 118] that the second largest (in magnitude) eigenvalue  $|\nu_2|$  of  $\mathcal{E}_k$  is less than 1, and its left-hand sides of decay as  $O(|\nu_2|^{-(k-j)})$ .

## Classification of 1D SPT phases

1D SPT phases are completely characterized by the degenerate edge states carrying projective representations of the symmetry group, i.e., there is a one-to-one correspondence between 1D SPT phases and the equivalence classes of projective representations. The edge states can be easily seen from the short-range correlated MPS representation (7.36) of SPT states. Suppose  $U$  is an on-site symmetry with the symmetry group  $G$ , i.e.,  $U$  is an isomorphism of  $G$  such that  $U(g)^{\otimes N}|\Psi\rangle = |\Psi\rangle$  for any  $g \in G$ . Recall that  $\{|i_k\rangle\}_{i_k=1}^d$  is the computational basis of the Hilbert space of the spin  $k$ . One can show that  $A_{i_k}^{(k)}$ 's satisfy [119, 29]

$$\sum_{i'_k} \langle i_k | U(g) | i'_k \rangle A_{i'_k}^{(k)} = e^{i\theta(g)} V_{k-1}(g) A_{i_k}^{(k)} V_k^{-1}(g), \quad (7.39)$$

as illustrated in Fig. 7.3(c). Furthermore,  $e^{i\theta(g)}$  is a 1D representation of  $G$ . It can be effectively eliminated by blocking sites unless  $G$  has an infinite number of 1D representations [29]; here we drop  $e^{i\theta(g)}$  for simplicity.  $V_k(g)$  is a projective representation of  $G$ . The equivalence class of  $V_k(g)$  is site independent and labels the SPT phase of the MPS  $|\Psi\rangle$ . As such, 1D SPT phases are classified by the second cohomology group  $H^2(G, U(1))$  in the presence of an on-site symmetry  $U$  [29, 136]. In particular, all 1D gapped spin systems are in the same phase in the absence of symmetry [29, 136], cf.  $H^2(G, U(1))$  is trivial if  $G$  is trivial.

1D SPT phases can be detected by nonlocal (string) order parameters. When the symmetry group  $G$  is Abelian, there is a set of string order parameters from which the SPT phase of any symmetric gapped ground state can be extracted [125, 103]. When  $G$  is not necessarily Abelian, a different and more complicated type of nonlocal order parameters fully characterizes SPT phases [55, 125].

## 7.8 Appendix: States in different phases

### Complete proof of Proposition 6

*Proof of Proposition 6.* We use the string order operator  $Q$  (7.10). Its expectation value  $\lim_{N \rightarrow +\infty} \langle Q \rangle$  is zero in the trivial phase and nonzero in the Haldane phase. As shown in Fig. 7.2,  $Q' = C^\dagger Q C = Q_l \prod_{j=N/3+m+1}^{2N/3-m-1} e^{i\pi S_j^y} Q_r$  remains a string (order) operator, where the end

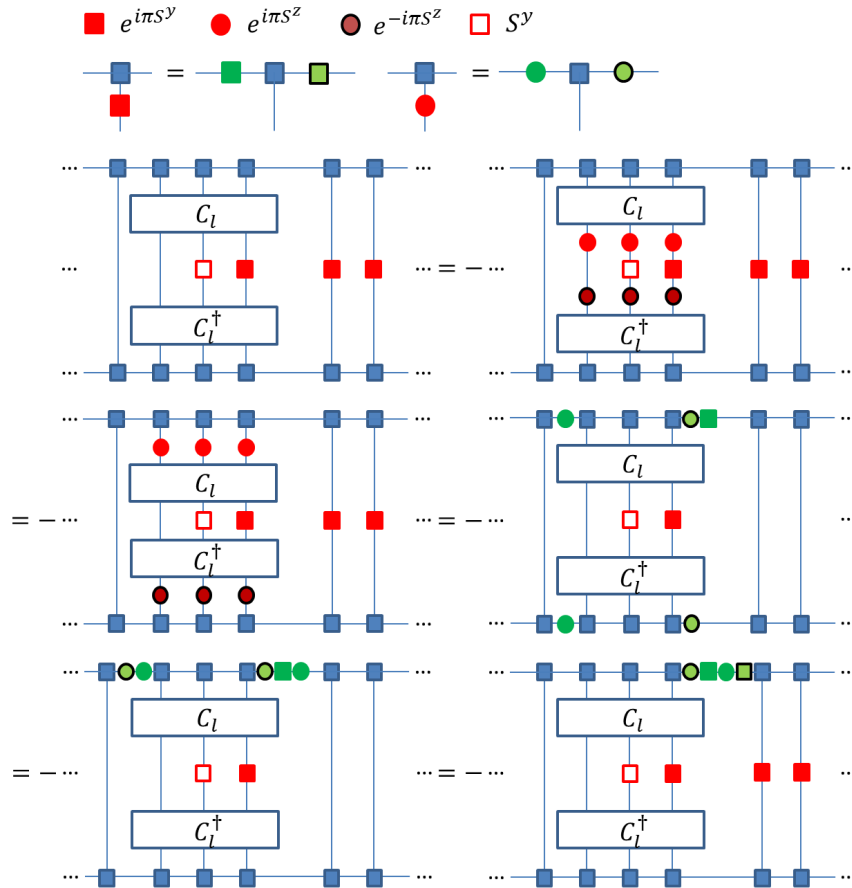


Figure 7.4: (Color online) Graphical proof of  $\langle \psi | Q' | \psi \rangle = 0$  in the thermodynamic limit  $N \rightarrow +\infty$  under the assumption that  $|\psi\rangle$  is in the trivial phase.

operators  $Q_l$  and  $Q_r$  are given by (7.11). It suffices to prove  $\lim_{N \rightarrow +\infty} \langle \psi | Q' | \psi \rangle = 0$  under the assumption that  $|\psi\rangle$  is in the trivial phase.

See Fig. 7.4 for a graphical proof. We focus on the left end of the string (order) operator  $Q'$ . The green squares and circles carry projective representations induced by the corresponding symmetry operators (red squares and circles, respectively). We briefly explain each step of the graphical equation chain:

Step 1:  $e^{-i\pi S^z} S^y e^{i\pi S^z} = -S^y$  and  $e^{-i\pi S^z} S^z e^{i\pi S^z} = S^z$ .

Step 2:  $C_l$  is symmetric.

Step 3: Figure 7.3(c).

Step 4: Figure 7.3(d).

Step 5: Figure 7.3(c).

In the last tensor network, the four green objects together contribute a trivial phase factor as  $|\psi\rangle$  is in the trivial phase. Therefore, the first tensor network is zero due to the minus signs in the graphical equation chain.  $\square$

## Linear depth

**Theorem 9.** *Suppose  $|\psi_0\rangle$  and  $|\psi_1\rangle$  are two symmetric gapped ground states in different SPT phases. Given an arbitrarily small constant  $\epsilon = \Theta(1)$ , there exist  $|\psi'_0\rangle, |\psi'_1\rangle$  and a symmetric local quantum circuit  $C$  of depth  $O(N)$  such that  $|\psi'_1\rangle = C|\psi'_0\rangle$  and*

$$|\langle\psi_k|P|\psi_k\rangle - \langle\psi'_k|P|\psi'_k\rangle| \leq \epsilon \quad (k = 0, 1) \quad (7.40)$$

for any local operator  $P$  with  $\|P\| \leq 1$ .

*Proof.* The proof proceeds analogously to that of Proposition 5. Assume without loss of generality that  $|\psi_k\rangle$  is in a nontrivial SPT phase. Let  $|\phi\rangle$  be the RG fixed-point state in the trivial SPT phase, and  $|\phi_k\rangle$  be the RG fixed-point state in the same SPT phase as  $|\psi_k\rangle$ . Figure 7.1(a) and (b) illustrate the structures of  $|\phi\rangle$  and  $|\phi_k\rangle$ , respectively.

As shown in Fig. 7.1(c),  $|\phi\rangle$  and  $|\phi_k\rangle$  can be exactly mapped to each other by applying  $O(N)$  2-local SWAP gates sequentially. These SWAP gates are symmetric with respect to any on-site symmetry and form a symmetric 2-local quantum circuit  $C_{\phi,k}$  of depth  $O(N)$ . As  $|\psi_k\rangle$  and  $|\phi_k\rangle$  are in the same SPT phase, there exists a symmetric local quantum circuit  $C_k$  of depth  $O(1)$  (Corollary 4) such that  $|\langle\psi_k|P|\psi_k\rangle - \langle\psi'_k|P|\psi'_k\rangle| \leq \epsilon$  for any local operator  $P$  with  $\|P\| \leq 1$ , where  $|\psi'_k\rangle = C_k|\phi_k\rangle$ . Finally,  $C = C_1 C_{\phi,1} C_{\phi,0}^\dagger C_0^\dagger$  is the symmetric circuit of linear depth that connects  $|\psi_0\rangle$  and  $|\psi_1\rangle$ .  $\square$

## Linear lower bound

The proof of Proposition 6 can be generalized to other Abelian on-site symmetry. Indeed, string order parameters do (do not) fully characterize 1D SPT phases with Abelian (non-Abelian) on-site symmetry [125, 103]. When the symmetry group is not necessarily Abelian, a different and more complicated type of nonlocal order parameters [55, 125] measures all gauge-invariant phase factors, which provide a complete description of the equivalence class of projective representations.

**Theorem 10.** *Suppose  $|\psi\rangle$  and  $C|\psi\rangle$  are two symmetric gapped ground states in 1D spin systems with an on-site symmetry  $U$ , where  $C$  is a symmetric local quantum circuit of sub-linear depth. Then  $|\psi\rangle$  and  $C|\psi\rangle$  are in the same SPT phase.*

*Proof.* As gauge-invariant phase factors provide a complete description of the equivalence class of projective representations, it suffices to show that all gauge-invariant phase factors cannot change under symmetric local quantum circuits of sub-linear depth. Let  $V$  be the projective representation of the symmetry group  $G$  that labels the SPT phase of  $|\psi\rangle$ . The simplest example of a gauge-invariant phase factor is  $V(g_1)V(g_2)V^{-1}(g_1)V^{-1}(g_2)$  for  $g_1, g_2 \in G$  with  $U(g_1)U(g_2)U^{-1}(g_1)U^{-1}(g_2) = 1$ . However, the graphical representation of the nonlocal order parameter that measures this gauge-invariant phase factor contains eight copies of  $|\psi\rangle$  and is cumbersome. In order to simplify the illustration of our proof, we pretend that  $V(g_1)V(g_2)$  with  $U(g_1)U(g_2) = 1$  is a gauge-invariant phase factor so that the

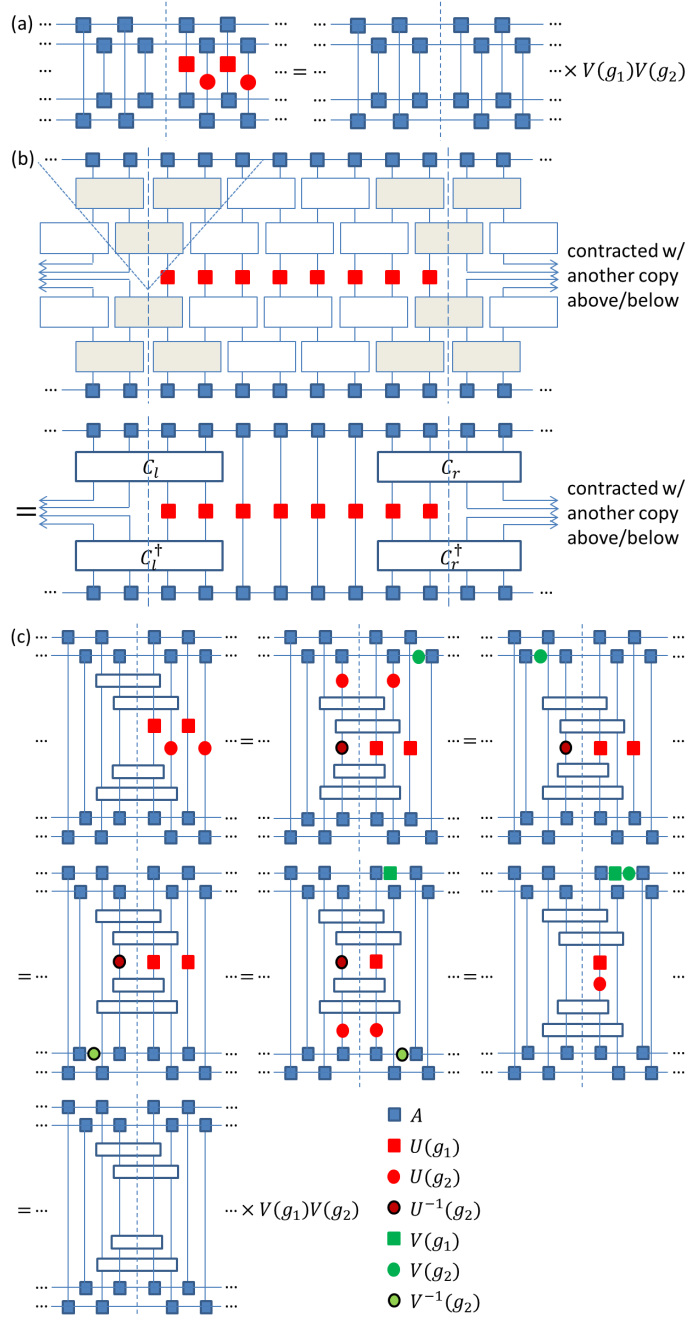


Figure 7.5: (Color online) (a) The domain wall (dashed line) that contributes the local phase factor  $V(g_1)V(g_2)$  [125]. (b) The short rectangles are the local unitaries in  $C$ . The (white) unitaries outside the causal cones (dotted lines) of the domain walls can be removed, as they are symmetric. Then we merge the (gray) symmetric local quantum gates inside each causal cone into one symmetric quantum gate (long rectangle) of sub-linear support. (c) Graphical proof of the invariance of the local phase factor for the domain wall in (a) under symmetric local quantum circuits of sub-linear depth.

corresponding nonlocal order parameter contains only four copies of  $|\psi\rangle$ . We show that this “gauge-invariant phase factor” cannot change under symmetric local quantum circuits of sub-linear depth. It is straightforward to generalize the proof to any gauge-invariant phase factor.

We briefly review the construction of the tensor network (nonlocal order parameter) that measures the gauge-invariant phase factor  $V(g_1)V(g_2)$ . The tensor network contains three domain walls. As  $|\psi\rangle$  is short-range correlated in the sense of (7.38), one can define a “local phase factor” for each domain wall such that the overall phase factor is the product of all three local phase factors. Specifically, the domain wall in Fig. 7.5(a) contributes the local phase factor  $V(g_1)V(g_2)$ . The other two domain walls (not shown) are  $\Theta(N)$  sites away; they do not contribute any nontrivial local phase factors, but are necessary for restoring periodic boundary conditions. The left-hand side of the graphical equation in Fig. 7.5(a) is constructed as follows. We take four copies of  $|\psi\rangle$  (expressed as MPS): two copies above and two copies below [tensors in the copies below are complex conjugated]; contract them via a permutation to the left and via the symmetry operators  $U(g_1), U(g_2)$  (red squares and circles) to the right of the domain wall. Then the local phase factor  $V(g_1)V(g_2)$  pops out, as illustrated in Fig. 7.5(a).

Under symmetric local quantum circuits of sub-linear depth, Fig. 7.5(b) shows that the local phase factor for each domain wall is still well defined and Fig. 7.5(c) proves its invariance. Specifically, in Fig. 7.5(c) we assume without loss of generality that  $C$  is a symmetric 2-local quantum circuit of depth 1 so that all four rectangles [corresponding to the gates  $C_l$  and  $C_l^\dagger$  in Fig. 7.5(b)] in each tensor network are symmetric and 2-local. The first (from above to below) rectangle acts on the third and fifth (from left to right) vertical lines; the second acts on the fourth and sixth; the third acts on the fourth and fifth; the fourth acts on the third and sixth. All other crossings between rectangles and vertical lines should not be there if we could draw the tensor networks in 3D rather than in 2D. We briefly explain each step of the graphical equation chain:

Step 1: Figure 7.3(c) and the symmetry of the rectangles.

Step 2: Figure 7.3(c).

Step 3: Figure 7.3(d).

Step 4: Figure 7.3(c).

Step 5: Figure 7.3(d) and the symmetry of the rectangles.

Step 6:  $U(g_1)U(g_2) = 1$ . □

*Remark.* The time-reversal symmetry is not an on-site symmetry as the anti-unitary time-reversal operator cannot be expressed as a tensor product of on-site operators. However, it can be effectively treated as an on-site symmetry using the trick in Sec. IVB of Ref. [125]. Therefore, we expect that the proof of Theorem 10 can be generalized to the time-reversal symmetry.

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