Investigation on 1D Area Law and XXZ Model

A Thesis

Presented to

The Division of Mathematics and Natural Sciences

Reed College

In Partial Fulfillment

of the Requirements for the Degree

Bachelor of Arts

Kaiyan Shi

May 2020

Approved for the Division
(Mathematics and Computer Science)

Jamie Pommersheim	Adam Groce

Acknowledgements

Thank you...

To my parents and grandparents, thank you very much for supporting me for over twenty years.

To Professor Jamie Pommersheim, thank you for being my thesis advisor and providing me constructive advice for my thesis. Thank you for leading me to quantum computation.

To Professor Adam Groce, thank you for guiding me to both computer science and research. Thank you for being so supportive for these four years.

To all professors who have taught me at Reed and BSM, thank you for being role models whom I would love to learn from. Thank you for all the encouragement and suggestions given to me.

To all friends I have met at Reed and BSM, thank you for accompanying me for these wonderful and colorful four years. Thank you for all the time studying and relaxing together.

To all friends I have met outside of Reed, thank you for always being with me for another four years.

Contents

Introduction **1**
0.1 Why study Area Law? 1

Chapter 1: Introduction to Quantum Computation **3**
1.1 Quantum Bits 3
1.2 Composite Systems 3
1.3 The Schmidt Decomposition 4
1.4 Entanglement Entropy 5

Chapter 2: Introduction to Area Law **7**
2.1 Brief Introduction 7
2.2 Related Work 7
2.3 Proof of 1D Area Law 8
2.3.1 High-Level Overview 8
2.3.2 Prelimaries: AGSP 9
2.3.3 Good AGSP with good product state implies 1D area law 10
2.3.4 Good AGSP implies a good product state 14
2.3.5 Construction of AGSP 15
2.4 Discussion of Frustrated Hamiltonian 21
2.5 Discussion of Degenerate Ground States 22

Chapter 3: Introduction to Quantum Models **23**
3.1 XXZ Model 23
3.2 XXZ-Variant Model 25
3.3 AKLT Model 25

Chapter 4: Numerical Techniques to Study Physical Models **27**
4.1 Standard Construction 27
4.2 Quicker Construction based on Hamming Weights 28
4.3 Construction by Density Matrix Renormalization Group 31
4.3.1 Brief Introuction 31
4.3.2 Single Enlargement and Truncation in DMRG 32
4.3.3 The Infinite and Finite System DMRG 37

Chapter 5: Area Law on Quantum Models **39**
5.1 XXZ Model 39
5.1.1 Entropy Entanglement vs. Position of the Cut 39
5.1.2 Entropy Entanglement vs. Number of Qubits 40
5.1.3 Schmidt Coefficients Value Distribution 42
5.2 XXZ-Variant Model 46
5.2.1 Entropy Entanglement vs. Number of Qubits 46
5.3 AKLT Model 47
5.3.1 Entropy Entanglement vs. Number of Qubits 47

Chapter 6: Quasi-Approximate Ground State Projector **49**
6.1 Construction of QAGSP 49
6.1.1 Frustration Free: $a = 0$ 50
6.1.2 Positive Ground State Energy: $a > 0$ 50
6.1.3 Negative Ground State Energy: $a < 0$ and $|a| < b$ 50
6.1.4 Negative Ground State Energy: $a < 0$ and $|a| > b$ 51
6.2 Ground State Convergence 51
6.3 Schmidt Coefficients Value Distribution 52
6.3.1 Theory on Number of Non-Zero Schmidt Coefficients 52
6.3.2 Analysis on Schmidt Coefficients Value Distribution 54

Conclusion **57**
4.1 Possible Improvements 57

Appendix A: Schmidt Coefficients Value Distribution for Larger Δs **59**

Appendix B: Code **61**

Bibliography **63**

List of Tables

4.1 Parameters for Implementation of Algorithm 3 29

6.1 t vs. n such that K^t is a QAGSP 51

List of Figures

2.1 A 1D quantum system with surface area = 1. 8
2.2 A 1D quantum system with surface area = 2. 8
2.3 The Schmidt Rank of Each Term across the Middle Cut. 20

5.1 Entropy Entanglement vs. Position of the Cut for XXZ Model 40
5.2 Entropy Entanglement vs. Number of Qubits for XXZ Model with $1 < \Delta < 99$ 41
5.3 Entropy Entanglement vs. Number of Qubits for XXZ Model with $\Delta \longrightarrow \infty$ 41
5.4 Schmidt Coefficients Value Distribution for XXZ Model with $\Delta = 5$ 42
5.5 The Slope of Schmidt Coefficients Value Distribution vs. Number of Qubits for XXZ Model 43
5.6 The Slope of Schmidt Coefficients Value Distribution vs. Number of Qubits for XXZ Model with $\Delta = 5$ 44
5.7 The Predicted and Real Slope of Schmidt Coefficients Value Distribution vs. Δ for XXZ Model with $n = 5$ 45
5.8 Entropy Entanglement vs. Number of Qubits for XXZ Variant Model 46
5.9 Entropy Entanglement vs. Number of Qubits for AKLT Model 47

6.1 Entanglement Entropy vs. t for QAGSP of XXZ Model with $\Delta = 5$ 52
6.2 Schmidt Coefficients Value Distribution of QAGSP for XXZ Model with $\Delta = 5$ 54
6.3 The Slope of Schmidt Coefficients Value Distribution of QAGSP vs. t for XXZ Model 55
6.4 The Slope of Schmidt Coefficients Value Distribution of QAGSP vs. n for XXZ Model at $t = 10$ 55

A.1 Schmidt Coefficients Value Distribution for XXZ Model with $\Delta = 15$ 59
A.2 Schmidt Coefficients Value Distribution for XXZ Model with $\Delta = 20$ 60

Abstract

An area law is investigated and verified for the von Neumann entanglement entropy of ground states in XXZ model, up to 14 qubits. The Schmidt coefficients of ground states of XXZ model with up to 13 qubits appear to be distributed exponentially. Slopes are studied to predict the slope of the Schmidt coefficients distribution of 14 qubits, and discrepancies are within 0.1 for $2 \leq \Delta \leq 80$. Quasi-approximate ground state projectors K^t that can map random product states to ground states are also studied and Schmidt coefficients of $K^t |\psi\rangle$ also appear to be distributed exponentially up to 10 qubits.

Introduction

In this thesis, we investigate area laws in quantum computation, i.e. under certain conditions, the amount of entanglement between a subsystem and its complement grows as the *surface area or the boundary* and this is why these laws are called area laws. We focus on one-dimensional(1D) area law, i.e. the amount of entanglement between a subsystem and its complement is $\mathcal{O}(1)$ because in 1D, the surface area is a constant.

In Chapter 1, we introduce relevant quantum concepts that are useful in understanding 1D area law, including von Neumann entropy which is the measurement of entanglement we use in this thesis.

In Chapter 2, we review a combinatorial proof [3] of Hastings' 1D area law [17] with more detailed explanation. Chapter 3 introduces models we are interested in investigating 1D area law on: the XXZ model, the XXZ Variant model and the AKLT model. Chapter 4 states three algorithms which we can use to compute entanglement entropy of the ground state of a certain model.

Then with all these preliminaries given, we investigate entanglement entropy growth for these introduced models in Chapter 5 to verify the 1D area law. The distribution of Schmidt coefficients of the ground state is also studied to investigate the relationship between Schmidt coefficients and number of qubits.

In the last chapter, Chapter 6, we introduce the Quasi-Approximate Ground Sate Projector K^t, which aims to map a random product state $|\psi\rangle = |A\rangle \otimes |B\rangle$ to the ground state of the studied system. We then study Schmidt coefficients distribution of $K^t |\psi\rangle$ which might be beneficial to deduce the Schmidt coefficients for larger number of qubits.

0.1 Why study Area Law?

In classical description, properties of a quantum system are in general associated with the exponential of the number of qubits. But area laws provide a way to describe some properties of a quantum system polynomially. In particular, area laws play an important role in the study of the complexity of ground states in that they provide quantitative bounds on the entanglement entropy, and such bounds do not grow exponentially with number of qubits.

As for 1D area law, we would like to understand it well in order to get a better chance of establishing area laws in higher dimensions, for which little is known.

It is necessary to study entanglement entropy for the 1D area law, but at the same time, we also study the Schmidt coefficients value distribution. The reason is that for a system of n qubits, if its ground state's 2^n Schmidt coefficients follow a certain distribution, then we can obtain a formula for approximating the entanglement entropy. We can just generate 2^n numbers from the function and treat them as Schmidt coefficients to calculate entanglement entropy. Calculation of entropy in this way will not involve generating the Hamiltonian which costs a great deal of computation time. Also from a theoretical point of view, if the distribution exists, we might obtain a different proof or a better understanding of existing proofs. So such investigation would be very beneficial for investigating area law in general.

As for the QAGSP, given a product state $|\psi\rangle$, with t increases, K^t will map $|\psi\rangle$ gradually to the ground state. We study the entropy convergence to see at which t, the entropy starts to be stable. We also study the Schmidt coefficients value distribution to see how they change with t and how we might use the relationship to predict Schmidt coefficients of $K^t |\psi\rangle$ with t being very large, which is essentially the ground state. This also aims to save computation time to investigate area law.

Chapter 1

Introduction to Quantum Computation

The paper focuses on 1D area Law, which is a theorem about entanglement entropy of quantum models. In this section, we introduce some basic concepts and knowledge about quantum computation [22].

1.1 Quantum Bits

Just as a classical bit has a state - either 0 or 1 - a qubit also has a state. States a qubit can have are the states $|0\rangle$ and $|1\rangle$, which can be considered just as different notations of classical states. The difference is that a qubit can be in a state which is a superposition of $|0\rangle$ and $|1\rangle$. We usually write a qubit in the following way:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,,$$

where α and β are complex numbers. Also we always require qubit written in a normalized form, i.e. $|\alpha|^2 + |\beta|^2 = 1$.

1.2 Composite Systems

In this thesis, we are usually concerned with a composite quantum system made up of two (or more distinct physical systems). The following postulate given in [22] describes how the state space of a composite system is built up from the state spaces of the component systems:

Postulate 1.2.1. *The state space of a composite physical system is the tensor product of the component physical systems. Moreover, if we have systems numbered* 1 *through* n*, and system number* i *is prepared in the state* $|\psi_i\rangle$*, then the joint state of the total system is* $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \ldots \otimes |\psi_n\rangle$ *.*

A bipartite system is a composite system consists of 2 components, and states in such system usually denoted as $|\psi_1\rangle \otimes |\psi_2\rangle = |\psi_1\rangle\,|\psi_2\rangle$. For our purpose, it is useful to mention

a meaningful subscript notation to denote states and operators on different systems. Still take the bipartite system as an example,

$$\begin{aligned} X_1 Y_2 \left|\psi_1\right\rangle \left|\psi_2\right\rangle &= \left(X \otimes \mathbb{I}\right)\left(\mathbb{I} \otimes Y\right)\left|\psi_1\right\rangle \left|\psi_2\right\rangle \\ &= \left(X \otimes \mathbb{I}\right)\left(\mathbb{I}\left|\psi_1\right\rangle \otimes Y\left|\psi_2\right\rangle\right) \\ &= X\mathbb{I}\left|\psi_1\right\rangle \otimes \mathbb{I}Y\left|\psi_2\right\rangle \\ &= X\left|\psi_1\right\rangle \otimes Y\left|\psi_2\right\rangle \end{aligned}$$

where X and Y are some operators acting on a single qubit.

1.3 The Schmidt Decomposition

Here we give theorems that are useful for our investigation on 1D area law. Schmidt decomposition is the basis of von Neumann entropy calculation and singular value decomposition is useful for the proof and computation of Schmidt decomposition. So we will introduce these two theorems here with their proofs.

Theorem 1.3.1. *(Singular value decomposition) Let A be a square matrix. Then there exist unitary matrices U and V, and diagonal matrix D with non-negative entries such that*

$$A = UDV.$$

The diagonal elements of D are called the singular values of A.

Proof.

By the polar decomposition (Theorem 2.3 in [22]), A can be written in the form $A = SJ$, for unitary S, and positive J. By the spectral theorem, $J = TDT^\dagger$, for unitary T and diagonal D with non-negative entries. Setting $U \equiv ST$ and $V \equiv T^\dagger$ completes the proof.

End of proof.

We now introduce Schmdit decomposition, in which singular value decomposition is used.

Theorem 1.3.2. *(Schmidt decomposition) Suppose $\left|\psi\right\rangle$ is a pure state of a composite system, AB. Then there exist orthonormal states $\left|i_A\right\rangle$ of system A and orthonormal states $\left|i_B\right\rangle$ of system B such that*

$$\left|\psi\right\rangle = \sum_i \lambda_i \left|i_A\right\rangle \left|i_B\right\rangle,$$

where λ_i are non-negative real numbers satisfying $\sum_i \lambda_i^2 = 1$ known as Schmidt coefficients.

Proof.

Let A and B be two systems of the same size, with $|j\rangle$ and $|k\rangle$ being their fixed orthonormal bases for them respectively. Suppose $|\psi\rangle$ is a pure state of the composite system, $A \otimes B$ and then it can be written

$$|\psi\rangle = \sum_{jk} a_{jk} |j\rangle |k\rangle ,$$

for some matrix a of complex numbers a_{jk}. By the singular value decomposition, $a = udv$, where d is a diagonal matrix with non-negative elements, and u and v. Thus

$$|\psi\rangle = \sum_{ijk} u_{ji} d_{ii} v_{jk} |j\rangle |k\rangle .$$

Defining $|i_A\rangle \equiv \sum_j u_{ji} |j\rangle$, $|i_B\rangle \equiv \sum_k v_{ik} |k\rangle$, and $\lambda_i \equiv d_{ii}$, we see that this gives

$$|\psi\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle .$$

From the unitarity of u and the orthonomality of $|j\rangle$, we can see that $\{|i_A\rangle\}$ form an orthonormal set, and it is the similar argument for $\{|i_B\rangle\}$.

End of proof.

Note that singular value decomposition is not unique. It is always possible to choose the decomposition so that the singular values d_{ii} are in descending order. In this case, D (but not always U and V) is uniquely determined by A. It then follows that Schmidt decomposition in general is also not unique, but $\{\lambda_i\} = d_{ii}$ is unique.

We also define the Schmidt rank of an operator here, whose concepts are similar as Schmdit numbers.

Definition 1. *Given an operator A, its Schmidt rank is defined as the smallest integer m such that A can be written in the form*

$$A = \sum_{1 \le i \le m} L_i \otimes R_i.$$

1.4 Entanglement Entropy

There is an entire field of research on how to measure entanglement entropy in quantum many body systems. Von Neumann entropy is a frequently used way of measurement, and it is also the one used in the proof of 1D area law which we will discuss in Section 2.

The von Neumann entropy is used to measure the entanglement between two components of the system. Consider a composite quantum system consisting of A and B with the Hamiltonian $H = H_A \otimes H_B$, where a *Hamiltonian* is a matrix that represents the sum of kinetic

energies of all qubits, together with the potential energy of the qubits associated with the system.

We then take a state $|\psi_{AB}\rangle$. After Schmidt decomposing the state $|\psi_{AB}\rangle$, we will get

$$|\psi_{AB}\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle .$$

The von Neumann entropy between these bi-partitions is defined as

$$S_A = S_B = -\sum_i \lambda_i^2 \log \lambda_i^2,$$

which is a proper extension of the classical Shannon entropy [26] to the quantum case,

Chapter 2

Introduction to Area Law

2.1 Brief Introduction

Roughly, an *area law* states that for certain interesting classes of quantum many-body systems, the amount of entanglement between a subsystem and its complement grows as the *surface area or the boundary* rather than the *volume* of the subsystem. In the literature, the amount of entanglement entropy is typically formulated as entanglement entropy, i.e. the von Neumann entropy of the reduced density matrix of the subsystem of interest.

As stated in the introduction, an area law plays an important role in the study of the complexity of ground states in the way that it provides bounds quantitatively on the entanglement entropy. In 1D, such bound is irrelevant to the number of qubits. So here we would like to give a review of the proof of 1D area law, which we will invesigate by examples in Chapter 5.

2.2 Related Work

For the critical or gapless systems, many constructions are known to violate the area law. ([4], [16], [19], [24] and [10]). People usually show a high degree of quantum entanglement in the ground state of a system to demonstrate ground state complexity and prove the complexity of a class of problems. Therefore verifying that the area laws fail is also important for the development the whole area. But in this thesis, we focus on the verification of the area law.

In this section, we review a combinatorial proof [3] of Hastings' 1D area law [17]. A more understandable and structured explnation of the combinatorial proof of 1D area law is shown in [15]. The structure of the proof I will show below mainly follows Section 7.5 in [15], but will also combine some proofs in [6] and in several places, I will add more detailed explanations.

Figure 2.1: A 1D quantum system with surface area = 1.

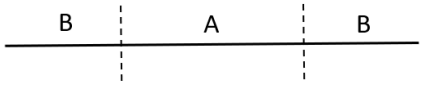

Figure 2.2: A 1D quantum system with surface area = 2.

There is also some recent work which proves that the entanglement entropy of the ground state of 2D frustration-free spin systems is upper bounded by $\mathcal{O}(L^{\frac{5}{3}})$, where L is the number of qubits in a subsystem [5].

2.3 Proof of 1D Area Law

2.3.1 High-Level Overview

We present Arad, Kitaev, Landau and Vazirani's combinatorial proof [6] of Hastings' [17] 1D area law for gapped systems. Specifically, we consider a 1D chain of n qubits governed by a gapped local Hamiltonian H. Any state of this quantum system lies in the Hilbert space $\mathbb{C}^2 \otimes \ldots \otimes \mathbb{C}^2$.

A *$k-$local Hamiltonian* is the sum of Hamiltonians, each of which act non-trivially on at most k adjacent qubits instead of all n qubits. The value of k we use in the rest of the chapter depends on the subsystem we focus on.

By *gapped*, we mean that the difference between the smallest and second-smallest eigenvalues of H is bounded below by a constant $\epsilon \geq 0$. We also assume that the ground state is unique (See Section 2.5 for non-unique ground states).

In the following sections, we prove that there exists an area law for 1D gapped systems. By definition the surface area of any contiguous region in a 1D system must be constant (i.e. the number of 'cutting points' of lines, and so either 1 (Figure 2.1) or 2 (Figure 2.2)). It follows that to prove 1D area law, it suffices to prove that

In the ground state, for any $1 \leq i \leq n$, the entanglement entropy between particles $1, \ldots, i$ and particles $i+1, \ldots, n$ is bounded above by a constant.

Here, the entanglement entropy is defined as the von Neumann entropy of the reduced density matrix on particles $1, \ldots, i$. Without loss of generality, it suffices to fix an arbitrary cut and prove the statement above; In the following parts, let C denote this cut.

Conceptually, the proof has two components. First, we show that there exists a product state with respect to cut C which has reasonably good, i.e. constant, overlap with the ground state of H. Second, we 'transform' such a product state to a much better approximation of the

ground state without increasing the entanglement entropy across C too much. Both of these components depend crucially on a theoretical construct called an *Approximate Ground-Space Project (AGSP)*, with good parameters.

For simplicity, in this review, we only focus on frustration-free Hamiltonians, whose ground state energy is 0. The frustrated case is discussed is Section 2.4.

We proceed by the following procedures:

1. In Section 2.3.3, we prove that the existence of a good AGSP and a good product state, i.e. non-trivial overlap with the ground state of H, implies the area law.
2. In Section 2.3.4, we prove that, actually, the existence of a good AGSP already implies a good product state. Note that 1D Area Law is stated in Theorem 2.3.3.
3. In Section 2.3.5, we constructs a good AGSP, which finishes the 1D Area Law proof.

2.3.2 Prelimaries: AGSP

From Section 2.3.1, we would like to "transform" a good product state to a much better approximation of the ground state without increasing entanglement entropy C too much. In other words, we want a projection to map $|\psi_{\text{prod}}\rangle$, with non-trivial overlap with the ground state of $\hat{H}$, to a good approximation of the ground state.

The obvious projection is $|\psi_{\text{ground}}\rangle \langle\psi_{\text{ground}}|$, such that when applied to $|\psi_{\text{prod}}\rangle$, we will obtain $\langle\psi_{\text{ground}} | \psi_{\text{prod}}\rangle |\psi_{\text{ground}}\rangle$, a scaled-down version of the ground state. However, applying this projection does not give a way to bound the amount of entanglement generated across cut C. Therefore, we would like to construct an *Approximate Ground-Space Project* AGSP to only approximately project onto the ground space; in return, we can obtain a rigorous bound on how the entanglement grows with the application of AGSP.

Here we give the definiton of AGSP.

Definition 2. *An operator K is said to be a (D, Δ)-AGSP if the following conditions hold:*

1. ***Ground space Invariance:*** *For any ground state $|\Gamma\rangle$, $K|\Gamma\rangle = |\Gamma\rangle$.*
2. ***Shrinking:*** *If $\left|\Gamma^{\perp}\right\rangle$ is any state orthogonal to the ground space, then $K\left|\Gamma^{\perp}\right\rangle$ is also orthogonal to the ground space, and moreover $||K\left|\Gamma^{\perp}\right\rangle||^2 \leq \Delta$.*
3. ***Entanglement:*** *The Schimidt rank of K across the given cut is at most D.*

If there exists an AGSP with small D and Δ, we can keep applying it to $|\psi_{\text{prod}}\rangle$ until we obtain a good approximation to the ground state. If the number of iterations goes to infinity, then the state will converge to the ground state. But a finite number of iterations provide a tradeoff between proximity to the ground state and a bound on the entanglement entropy.

2.3.3 Good AGSP with good product state implies 1D area law

Lemma 2.3.1 (Arad, Landau and Vazirani [6]). *Let $|\Gamma\rangle$ be the ground state of H and $|\phi\rangle$ a product state such that $|\langle\phi|\Gamma\rangle| = \mu$. Then, the existence of a (D, Δ)-AGSP K implies that the entanglement entropy S of $|\Gamma\rangle$ is bounded by*

$$S \leq O(1) \cdot \frac{\log \mu^2}{\log \Delta} \log D.$$

Proof. Let $|\Gamma\rangle = \sum_i \lambda_i |L_i\rangle \otimes |R_i\rangle$ be the Schmidt decomposition of the ground state $|\Gamma\rangle$, where the Schmidt coefficients λ_i. Then the entanglement entropy is defined by von Neumann entropy which is defined in Chapter 1.To bound this quantity, we consider the family of states $K^l |\phi\rangle$. By Definition 2, it follows that

1. The Schmidt rank of $K^l |\phi\rangle$ is at most D^l.

   Argument. By Definition 2, $K = \sum_{1 \leq i \leq D} L_i \otimes R_i$ and therefore $K|\phi\rangle$ can be written as at most D terms. $K^2|\phi\rangle = K(K|\phi\rangle)$ is at most D terms times D terms, which gives at most D^2 terms. By the same argument, we could say that the Schmidt rank of $K^l|\phi\rangle$ is at most D^l.

2. The inner product between normalized $K^l|\phi\rangle$ and $|\Gamma\rangle$ is at least $\frac{\mu}{\sqrt{\mu^2 + \Delta^l(1-\mu^2)}}$.

   Argument. We have conditions $|\langle\phi|\Gamma\rangle| = \mu$, and $||K\left|\Gamma^\perp\right\rangle||^2 \leq \Delta$. We then can write the product state in the basis of $|\Gamma\rangle$ and $\left|\Gamma^\perp\right\rangle$,

   $$|\phi\rangle = \pm\mu|\Gamma\rangle \pm \sqrt{1-\mu^2}\left|\Gamma^\perp\right\rangle.$$

   It follows that

   $$\begin{aligned} K|\phi\rangle &= \pm\mu K|\Gamma\rangle \pm \sqrt{1-\mu^2} K\left|\Gamma^\perp\right\rangle \\ &= \pm\mu|\Gamma\rangle \pm \sqrt{1-\mu^2} K\left|\Gamma^\perp\right\rangle. \end{aligned}$$

   Similarly, if we apply K l times, we will get

   $$\begin{aligned} K^l|\phi\rangle &= \pm\mu K^l|\Gamma\rangle \pm \sqrt{1-\mu^2} K^l\left|\Gamma^\perp\right\rangle \\ &= \pm\mu|\Gamma\rangle \pm \sqrt{1-\mu^2} K^l\left|\Gamma^\perp\right\rangle. \end{aligned}$$

   We now consider the normalization factor of this state. By the shrinking property in Definition 2, we have $||K^l\left|\Gamma^\perp\right\rangle||^2 = ||K^{l-1}K\left|\Gamma^\perp\right\rangle||^2 \leq ||K^{l-1}\left|\Gamma^\perp\right\rangle||^2\Delta \leq \Delta^l$, which leads to

   $$\begin{aligned} ||K^l|\phi\rangle||^2 &= \mu^2 + (1-\mu)||K^l\left|\Gamma^\perp\right\rangle||^2 \\ &\geq \mu^2 + \Delta^l(1-\mu^2) \end{aligned}$$

Therefore, we have the inner product between normalized $K^l |\phi\rangle$ and $|\Gamma\rangle$ is

$$\begin{aligned}\left|\langle\Gamma| \frac{K^l |\phi\rangle}{||K^l |\phi\rangle||}\right| &= \frac{|\langle\Gamma| K^l |\phi\rangle|}{||K^l |\phi\rangle||} \\ &= \frac{\mu \langle\Gamma|\Gamma\rangle}{||K^l |\phi\rangle||} \\ &\geq \frac{\mu}{\sqrt{\mu^2 + \Delta^l(1-\mu^2)}}.\end{aligned}$$

We then use these two properties to bound the entanglement entropy through the following two steps. The details of these two steps are not shown in [15].

1. $-\sum_{i\leq D^{4l_0}} \lambda_i^2 \log \lambda_i^2 \leq O(1) \cdot \frac{\log \mu^2}{\log \Delta} \log D$

   Argument. By the Eckart-Young theorem [11], which implies that the magnitute of the inner product between $|\Gamma\rangle$ and any normalizaed state with Schmidt rank r is upper bounded by the Euclidean norm of the vector of the first r Schmidt coefficients, i.e. by $(\sum_{i=1}^r \lambda_i^2))^{1/2}$. Therefore,

$$\begin{aligned}\sum_{i\leq D^l} \lambda_i^2 &\geq \left|\langle\Gamma| \frac{K^l |\phi\rangle}{||K^l |\phi\rangle||}\right|^2 \\ &\geq \frac{\mu^2}{\mu^2 + \Delta^l(1-\mu^2)} \\ &\geq \frac{\mu^2}{\mu^2 + \Delta^l},\end{aligned}$$

   where the first inequality follows from the Eckart-Young theorem. It follows that

$$\sum_{i> D^l} \lambda_i^2 \leq 1 - \frac{\mu^2}{\mu^2 + \Delta^l} = \frac{\mu^2}{\mu^2 + \Delta^l} = \frac{\Delta^l}{\mu^2 + \Delta^l} \leq \frac{\Delta^l}{\mu^2} =: p_l.$$

   We now choose $l_0 = \lceil \frac{\log \mu^2}{\log \Delta} \rceil$ so that $p_{l_0} = \frac{\Delta^{\lceil \frac{\log \mu^2}{\log \Delta} \rceil}}{\mu^2} = \frac{\Delta^{\lceil \log_\Delta \mu^2 \rceil}}{\mu^2} \leq \frac{\Delta^{\log_\Delta \mu^2}}{\mu^2} = 1$, where the inequality comes from the fact that $\Delta \leq 1$.

   Also it is easy to see that $\sum_{i\leq D^{4l_0}} \lambda_i^2 \leq 1$ as $\sum_i \lambda_i^2 = 1$ from Schmidt decomposition. So by the fact that the entropy of a (sub)normalized d-dimensional vector is at most $\log d$, we conclude that the contribution from the first D^{4l_0} Schmidt coefficients is at most

$$-\sum_{i\leq D^{4l_0}} \lambda^2 \log \lambda_i^2 \leq \log D^{4l_0} = 4l_0 \log D = O(1) \cdot \frac{\log \mu^2}{\log \Delta} \log D.$$

2. $-\sum_{i> D^{4l_0}} \lambda_i^2 \log \lambda_i^2 \leq \frac{\Delta}{(1-\Delta)^2} \log \frac{D^6}{\Delta}$

   Argument. First by previous argument, we have $p_{l_0} = \frac{\Delta^{l_0}}{\mu^2} \leq 1 \Rightarrow \Delta^{l_0} \leq \mu^2$. It follows

that $p_l = \frac{\Delta^l}{\mu^2} \leq \Delta^{l-l_0}$. Then we also have

$$\sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 \leq \sum_{i>D^{2l}} \lambda_i^2 \leq p_{2l} \leq p_l \leq \Delta^{l-l_0}.$$

It follows that $\sum_{i=D^{2l}+1}^{D^{2(l+1)}} \left(\frac{\lambda_i}{\sqrt{\Delta^{l-l_0}}}\right)^2 \leq 1$, which implies

$$\begin{aligned}
-\sum_{i=D^{2l}+1}^{D^{2(l+1)}} \frac{\lambda_i^2}{\Delta^{l-l_0}} \log \frac{\lambda_i^2}{\Delta^{l-l_0}} &\leq \log D^{2(l+1)} \\
\frac{1}{\Delta^{l-l_0}} \left(-\sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 \log \lambda_i^2 + \sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 \log \Delta^{l-l_0} \right) &\leq \log D^{2(l+1)} \\
-\sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 \log \lambda_i^2 + \log \Delta^{l-l_0} \sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 &\leq \Delta^{l-l_0} \log D^{2(l+1)} \\
-\sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 \log \lambda_i^2 - \left|\log \Delta^{l-l_0}\right| \sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 &\leq \Delta^{l-l_0} \log D^{2(l+1)} \\
-\sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 \log \lambda_i^2 &\leq \Delta^{l-l_0} \log D^{2(l+1)} + \left|\log \Delta^{l-l_0}\right| \sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 \\
-\sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 \log \lambda_i^2 &\leq \Delta^{l-l_0} \log D^{2(l+1)} + \left|\log \Delta^{l-l_0}\right| \Delta^{l-l_0} \\
-\sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 \log \lambda_i^2 &\leq \Delta^{l-l_0} \log D^{2(l+1)} - \log \Delta^{l-l_0} \Delta^{l-l_0} \\
-\sum_{i=D^{2l}+1}^{D^{2(l+1)}} \lambda_i^2 \log \lambda_i^2 &\leq \Delta^{l-l_0} (l-l_0) \log \frac{D^{2(l+1)/(l-l_0)}}{\Delta},
\end{aligned}$$

where the 4^{th} inequality comes from the fact that $\log \Delta^{l-l_0} \leq 0$.

We now consider the contribution from Schmidt coefficients other than the first D^{4l_0}.

$$\begin{aligned}
-\sum_{i>D^{4l_0}} \lambda^2 \log \lambda_i^2 &= -\sum_{j\geq 2l_0} \left(\sum_{i=D^{2j}+1}^{D^{2(j+1)}} \lambda_i^2 \log \lambda_i^2 \right) \\
&\leq \sum_{j\geq 2l_0} \Delta^{j-l_0}(j-l_0) \log \frac{D^{2(j+1)/(j-l_0)}}{\Delta} \\
&= \sum_{j\geq l_0} \Delta^j j \log \frac{D^{2(j+l_0+1)/j}}{\Delta} \\
&\leq \sum_{j\geq l_0} \Delta^j j \log \frac{D^6}{\Delta} \\
&\leq \left(\sum_{j\geq 1} \Delta^j j \right) \log \frac{D^6}{\Delta} \\
&= \frac{\Delta}{(1-\Delta)^2} \log \frac{D^6}{\Delta}.
\end{aligned}$$

where the fourth line comes from the fact that $\frac{j+l_0+1}{j} = 1 + \frac{l_0+1}{j} \leq 1 + \frac{l_0+1}{l_0} = 2\frac{1}{l_0} \leq 3$, and the last line comes from the series equality $\sum_{j\geq 1} jr^j = \frac{r}{(1-r)^2}$.

Combining the two bounds we have derived above, it follows that the entanglement entropy of the ground state satisfies

$$S = -\sum_i \lambda^2 \log \lambda_i^2 \leq O(1) \cdot \frac{\log \mu^2}{\log \Delta} \log D + \frac{\Delta}{(1-\Delta)^2} \log \frac{D^6}{\Delta}.$$

Finally, note that for any $k > 1$, it is easy to see that K^k is a $(D^k, \Delta^k) - AGSP$. Moreover, if we choose $k = \lceil -\frac{1}{\log \Delta} \rceil$, then we have

$$\log \Delta^k = \log \Delta^{\lceil -\frac{1}{\log \Delta} \rceil} = \lceil -\frac{1}{\log \Delta} \rceil \log \Delta \geq -1.$$

Therefore we can ensure that $\frac{1}{4} \leq \Delta^k \leq \frac{1}{2}$. Substituting D^k for D and Δ^k for Δ, we will obtain

$$\begin{aligned}
O(1) \cdot \frac{\log \mu^2}{\log \Delta^k} \log D^k &= O(1) \cdot k \cdot \log \mu^2 \frac{1}{\log \Delta^k} \log D \\
&\leq -O(1) \cdot k \cdot \log \mu^2 \log D,
\end{aligned}$$

and will also obtain

$$\begin{aligned}\frac{\Delta^k}{(1-\Delta^k)^2}\log\frac{D^{6k}}{\Delta^k} &\leq \frac{1/2}{(1-1/2)^2}k\log\frac{D^6}{\Delta}\\ &= 2k\cdot(6\log D-\log\Delta)\\ &= 12k\cdot\log D-2k\log\Delta\\ &= O(1)\cdot k\cdot\log D-O(1)\cdot k\cdot\log\Delta\\ &\leq O(1)\cdot k\cdot(\log D-1).\end{aligned}$$

Hence, we have

$$\begin{aligned}S &\leq O(1)\cdot k\cdot\left(-\log\mu^2\log D+\log D-1\right)\\ &= O(1)\cdot\left\lceil-\frac{1}{\log\Delta}\right\rceil\cdot\left(-\log\mu^2\log D+\log D-1\right)\\ &\leq O(1)\cdot\frac{\log\mu^2}{\log\Delta}\log D.\end{aligned}$$

End of proof.

2.3.4 Good AGSP implies a good product state

From Section 2.3.3, we know that to prove 1D area law, it suffices to have a good AGSP along with a product state with constant overlap with the ground state. In this section, we will show that actually a good AGSP will imply a good product state.

Lemma 2.3.2 (Arad, Landau and Vazirani [6])**.** *If there exists a $(D,\Delta)-AGSP$ K such that $D\cdot\Delta\leq\frac{1}{2}$, then there exists a product state $|\phi\rangle=|L\rangle\otimes|R\rangle$ whose overlap with the ground state $|\Gamma\rangle$ is $\mu=|\langle\Gamma|\phi\rangle|>\frac{1}{\sqrt{2D}}$.*

Proof. We prove the lemma by contradiction. Let $|\phi'\rangle$ be a product state such that $\langle\Gamma|\phi'\rangle\leq\mu$, and assume for sake of contradiction that $\mu<\frac{1}{\sqrt{2D}}$. Then, consider the state $|\phi\rangle:=\frac{K|\phi'\rangle}{||K|\phi'\rangle||}$. By definition of an AGSP, the Schmidt rank of $|\phi\rangle$ is at most D, and therefore it can be written as $|\phi\rangle=\sum_{i=1}^{D}\lambda_i|L_i\rangle\otimes|R_i\rangle$. It follows that

$$\begin{aligned}\frac{\mu^2}{||K|\phi'\rangle||^2} &= \frac{|\langle\Gamma|K|\phi'\rangle|^2}{||K|\phi'\rangle||^2}\\ &= |\langle\Gamma|\phi\rangle|^2\\ &\leq\left(\sum_{i=1}^{D}\lambda_i|\langle\Gamma|(|L_i\rangle\otimes|R_i\rangle)\rangle|\right)^2\\ &\leq\sum_{i=1}^{D}|\langle\Gamma|(|L_i\rangle\otimes|R_i\rangle)\rangle|^2,\end{aligned}$$

where the first equality comes from Definition 2 and the last inequality comes from Cauchy-Schwarz inequality, and $\sum_i \lambda_i^2 = 1$. Therefore there exists some i such that

$$|\langle\Gamma|(|L_i\rangle \otimes |R_i\rangle)\rangle|^2 \geq \frac{\mu^2}{||K|\phi'\rangle||^2} \geq \frac{\mu^2}{D(\mu^2+\Delta)},$$

where the last inequality follows from the fact that K is a (D,Δ)-AGSP and Definition 2. However by the assumption that $D\cdot\Delta \leq \frac{1}{2}$ and $\mu < \frac{1}{\sqrt{2D}}$, we know $D(\mu^2+\Delta) = D\mu^2 + D\Delta < \frac{1}{2}+\frac{1}{2} = 1$, which gives

$$|\langle\Gamma|(|L_i\rangle \otimes |R_i\rangle)\rangle| > \mu,$$

implying that $\langle\Gamma|(|L_i\rangle \otimes |R_i\rangle)\rangle$ has a larger overlap with $|\Gamma\rangle$ than $|\phi'\rangle$ does, and this raises a contraction. Therefore we should have $\mu > \frac{1}{\sqrt{2D}}$.

End of proof.

By combining Lemma 2.3.1 and 2.3.2, we obtain the following theorem.
Theorem 2.3.3 (1D Area Law)**.** *If there exists a (D,Δ)-AGSP such that $D\cdot\Delta \leq \frac{1}{2}$, the ground state entanglement entropy is bounded by $O(1)\cdot\log D$.*

2.3.5 Construction of AGSP

As Hamiltonian H is an operator which classifies a quantum system, we build a AGSP from H. For the quantum n-particle system under investigation, we consider a Hamiltonian H with the following structure: H_L acts on particle $1,\ldots,m$, $H = H_L + H_1 + H_2 + \ldots + H_s + H_R$, where H_i acts locally on particle $m+i$ and $m+i+1$, H_R acts on particle $m+s+1,\ldots,n$.

Assume that H has a unique ground state $|\Gamma\rangle$ with energy ϵ_0 ($\epsilon_0 = 0$ for frustration-free system) and that the other eigenvalues belong to the interval $[\epsilon_1, \|H\|]$. The spectral gap is $\epsilon = \epsilon_1 - \epsilon_0$, and we call a Hamiltonian gapped Hamiltonian if for an infinitely large many-body system, $\epsilon > 0$.

First Attempt: $K = I - \frac{H}{||H||}$

We need to construct an AGSP in this section, i.e. an operator that leaves the ground state invariant and shrinks every vector that is orthogonal to the ground state. As the only information regarding the ground state in our possession is the Hamiltonian H itself, we use H as our starting point. Consider the first attempt of operator of interest being $K = I - \frac{H}{||H||}$.

Note that H is a frustration-free Hamiltonian, which means that the ground state energy is zero. It also follows that the first excited state energy is ϵ, the spectral gap of the given Hamiltonian. Then it is easy to see that $K|\Gamma\rangle = |\Gamma\rangle - \frac{H|\Gamma\rangle}{||H||} = |\Gamma\rangle$, leaving the ground state invariant. As for the shrinking property, since $\frac{H|\Gamma^\perp\rangle}{||H||} \geq \frac{\epsilon}{||H||}|\Gamma^\perp\rangle$, K cuts the norm of any

orthogonal state to at most

$$\left|K\left|\Gamma^{\perp}\right\rangle\right| = \left|\left|\Gamma^{\perp}\right\rangle - \frac{H\left|\Gamma^{\perp}\right\rangle}{||H||}\right| \leq \left|\left|\Gamma^{\perp}\right\rangle - \frac{\lambda\left|\Gamma^{\perp}\right\rangle}{||H||}\right| \leq 1 - \frac{\epsilon}{||H||},$$

where λ is some energy level. Thus, K^k for large values of k yields an AGSP with a good value of Δ. Unfortunately, however, in general with this construction, since we raise K to the power of k and then its Schmidt rank will increase correspondingly, D will also grow exponentially in k. Thus, this candidate AGSP does not satisfy our required condition that $D \cdot \Delta \leq \frac{1}{2}$.

Second and Successful Attempt: $K = C_\ell(H)$

However, this first attempt leads us to consider manipulating the spectrum of H via matrix polynomials. We choose a polynomial $f(x)$ that maps 0 to 1 and $[\epsilon, \|H\|]$ to $[0, \Delta]$, and then as $\lambda_i \in [\epsilon, \|H\|]$, it follows that $f(\lambda_i) \in [0, \Delta]$. We then write an arbitrary vector $v \in \Gamma^{\perp}$ in terms of eigenvectors that are orthogonal to the ground state, $v = c_1 v_1 + \ldots$, which will give $Hv = \lambda_1 c_1 v_1 + \ldots$. Therefore by applying f, we will have

$$|f(H)v| = |f(\lambda_1)c_1 v_1 + \ldots| \leq |c_0 v_0 + \Delta(c_1 v_1 + \ldots)| = \Delta|v|,$$

which implies that $f(H)$ will have the shrinking factor Δ. Then the remaining task then is to show that $f(H)$ has a small Schmidt rank. Naturally one would expect that f must have a small degree, because the naive bound on the Schmidt rank grows at least exponentially in the degree of the polynomial.

Now it is the time to choose f. We consider the well-known family of polynomials T_ℓ called the **Chebyshev polynomial of the first kind** in approximation theory, which is defined by the recurrence relation:

$$\begin{aligned} T_0(x) &= 1 \\ T_1(x) &= x \\ T_{n+1}(x) &= 2xT_n(x) - T_{n-1}(x) \end{aligned}$$

It follows that it has the following properties [1]:

1. The degree of $T_\ell(x)$ is ℓ.
2. For $x \in [-1, 1], |T_\ell(x)| \leq 1$.
3. For $x > 1, T_\ell(x) \geq \frac{1}{2}e^{2\ell\sqrt{(x-1)/(x+1)}}$.

The main point is that once x passes the value 1, the polynomial begins to increase very rapidly, giving rise to a threshold-like behavior. We will use this behavior to address the challenge that the operator $f(H)$ should have an eigenvalue of 1 (as f maps 0 to 1) for the

ground state while it should have a very small eigenvalue for the first excited state which is only ϵ away from the ground state in the energy spectrum.

The strategy is to make the first excited state correspond to $T_\ell(1)$ and the largest eigenvector to $T_\ell(-1)$ so that all excited states have eigenvalues at most 1, (by property 2) while the ground state, which will then correspond to $T_\ell(1+y)$ for some small y has a much greater eigenvalue. Then we can renormalize the operator so that the eigenvalue of the ground state becomes 1, as required by the definition of an AGSP.

In other words, we construct a family of polynomials C_ℓ by scaling and translating T_ℓ as follows:

$$C_\ell(x) = T_\ell\left(\frac{\|H\| + \epsilon - 2x}{\|H\| - \epsilon}\right) / T_\ell\left(\frac{\|H\| + \epsilon}{\|H\| - \epsilon}\right).$$

It is easy to see that the numerator of $C_\ell(x)$ maps 0 to 1, ϵ to 0 and $\|H\|$ to -1. Then we can prove that $C_\ell(H)$ is an AGSP with $\Delta = 4e^{-4\ell\sqrt{\epsilon/\|H\|}}$. (We will use the fact that $P(\alpha + \beta H)v = P(\alpha + \beta\lambda)v$ where $Hv = \lambda v$.)

1. Ground space invariance:

   $C_\ell(H)\left|\Gamma\right\rangle = T_\ell\left(\frac{\|H\|+\epsilon-2H}{\|H\|-\epsilon}\right) / T_\ell\left(\frac{\|H\|+\epsilon}{\|H\|-\epsilon}\right)\left|\Gamma\right\rangle = T_\ell\left(\frac{\|H\|+\epsilon}{\|H\|-\epsilon}\right) / T_\ell\left(\frac{\|H\|+\epsilon}{\|H\|-\epsilon}\right)\left|\Gamma\right\rangle = \left|\Gamma\right\rangle$

2. Shrinking:

   We know that $\left|T_\ell\left(\frac{\|H\|+\epsilon-2x}{\|H\|-\epsilon}\right)\right| \leq 1$ for $x \in [\epsilon, \|H\|]$ as it maps $[\epsilon, \|H\|]$ to $[T_\ell(-1), T_\ell(1)]$. Therefore

   $$|C_\ell(x)| = \frac{\left|T_\ell\left(\frac{\|H\|+\epsilon-2H}{\|H\|-\epsilon}\right)\right|}{\left|T_\ell\left(\frac{\|H\|+\epsilon}{\|H\|-\epsilon}\right)\right|} \leq \frac{1}{\left|T_\ell\left(\frac{\|H\|+\epsilon}{\|H\|-\epsilon}\right)\right|} \leq \frac{1}{\frac{1}{2}e^{2\ell}\sqrt{\epsilon/\|H\|}} = 2e^{-2\ell\sqrt{\epsilon/\|H\|}},$$

   where the third inequality comes from that $\frac{\frac{\|H\|+\epsilon}{\|H\|-\epsilon}-1}{\frac{\|H\|+\epsilon}{\|H\|-\epsilon}+1} = \frac{\epsilon}{\|H\|}$, and then together with property 3 of T_ℓ that $T_\ell\left(\frac{\|H\|+\epsilon}{\|H\|-\epsilon}\right) \geq \frac{1}{2}e^{2\ell\sqrt{\epsilon/\|H\|}}$.

   Therefore we have, for $x \in [\epsilon, \|H\|]$,

   $$\begin{aligned}\left\|C_\ell(H)\left|\Gamma^\perp\right\rangle\right\|^2 &= \left\|C_\ell(x)\left|\Gamma^\perp\right\rangle\right\|^2 \\ &\leq \left(2e^{-2\ell\sqrt{\epsilon/\|H\|}}\right)^2 \\ &= 4e^{-4\ell\sqrt{\epsilon/\|H\|}}\end{aligned}$$

3. Entanglement: Proved by Lemma 2.3.4 using H' which is explained below.

However, as $\|H\|$ can be very large, the above bound on Δ will decay not as fast as expected. This issue can be addressed by a technique called *Hamiltonian truncation*. The technique

consists in picking out s particles around the cut and truncating the upper spectrum of the other 'less important' particles. As stated in the beginning of the section, we represent the Hamiltonian as $H = H_L + H_1 + \ldots + H_s + H_R$, where $\|H_1 + \ldots + H_s\| \leq s$, and H_L and H_R represents summation of Hamiltonian for particles not included in the s particles. The method used here is that we replace H_L and H_R by their respective truncated versions $H_L^{\leq t}$ and $H_R^{\leq t}$, where $A^{\leq t}$ denotes the matrix obtained from A by replacing all eigenvalues greater than t with t and leaving the other eigenvalues unchanged. Therefore considering the resulting truncated Hamiltonian H', we will see

$$\|H'\| = \sup|\lambda_{H_L} \leq t| + \|H_1 + \ldots + H_s\| + \sup|\lambda_{H_R} \leq t| \leq s + 2t.$$

It can also be shown that the spectral gap of H' remains to be $\Omega(1) \cdot \epsilon$ for $t = \mathcal{O}\left(\frac{1}{\epsilon}\right)$ (See [6] Lemma 6.1 for an explanation).

Moreover, since the Hamiltonian is frustration-free and gapped, H and H' have the same (unique by assumption) ground state. (This is the only time we use the constraint of frustration-free hypothesis in the whole proof.) This means that we can use H' in place of H in our construction of the AGSP because we only consider the ground state of the Hamiltonian here and then for $f(H')$, ground space invariance property follows directly. As the norm of H' is bounded up to our choice of s and t, we will have small enough Δ^k with not so large k, which will make the shrinking property of $C_\ell(H')$ and then $C_\ell(H)$.

We now need to prove that $C_\ell(H')$ has a small Schmidt rank across the given cut to make it an acceptable AGSP.

Lemma 2.3.4. *The Schmidt rank of $K = C_\ell(H')$ across the middle cut is bounded by $D = (d\ell)^{\mathcal{O}(\ell/s)}$. [6]*

Proof. W.l.o.g we may assume that $s \leq \sqrt{l}$. If this is not the case, we can reduce s to $\sqrt{\ell}$ by joining some of the H_j's with either H_L or H_R. This does not change the actual entanglement rank or the required bound. After this reduction, $s \leq \sqrt{l}$.

By the property of T_ℓ, and then C_ℓ, each term in the expansion of $C_\ell(H')$ is a product of at most ℓ terms of H'. We will bound the Schmidt rank added by each term, and so it suffices to analyze the Schmidt rank of the worst case $(H')^\ell$. We first consider the expansion

$$(H')^\ell = \left(H_L^{\leq t} + H_1 + \ldots H_s + H_R^{\leq t}\right)^\ell = \sum_{j_1,\ldots,j_\ell} H_{j_1} \ldots H_{j_\ell},$$

where as explained before, H_i acts locally on particle $m+i$ and $m+i+1$, H_L acts on particle $1, \ldots, m$, H_R acts on particle $m+s+1, \ldots, n$ and the summation is over all products of ℓ Hamiltonians from the set $\left\{H_L^{\leq t}, H_1, \ldots H_s, H_R^{\leq t}\right\}$. However it has exponentially many terms in the expansion and thus we cannot simply evaluate each term and sum these up. So we circumvent this problem by cleverly grouping the exponential number of terms by the

number of occurrences of each H_j. To this end, we introduce a generating function, which is a polynomial in a formal commuting variables $Z_0, \dots Z_{s+1}$:

$$P_\ell(Z) = (H_L Z_0 + H_1 Z_1 + \cdots + H_R Z_{s+1})^\ell = \sum_{a_0+\cdots+a_{s+1}=\ell} f_{a_0,\dots,a_{s+1}} Z_0^{a_0} Z_1^{a_1} \dots Z_{s+1}^{a_{s+1}},$$

where $f_{a_0,\dots,a_{s+1}}$ is the sum of products $H_{j_1} \dots H_{j_\ell}$, where each H_j occurs exactly a_j times. Note that we are interested in estimating the Schmidt Rank of $(H')^\ell = \sum_{j_1,\dots,j_\ell} H_{j_1} \dots H_{j_\ell} = \sum_{a_0+\cdots+a_{s+1}=\ell} f_{a_0,\dots,a_{s+1}}$.

We start by noticing that for each multi-index $(a_0, \dots, a_{s+1})$, there is some $i \in \{1, \dots, s\}$ such that $a_i \le \ell/s$ by pigeonhole principle. Thus,

$$(H')^\ell = \sum_{k=0}^{\ell/s} Q_{1,\ell k} + \ldots + \sum_{k=0}^{\ell/s} Q_{s,\ell k} = \sum_{i=1}^{s} \sum_{k=0}^{\ell/s} Q_{i,\ell k},$$

where $Q_{i,\ell k}$ is the sum of operators such that $a_i = k$ and $\sum_{j\neq i} a_j = \ell - k$. (This decomposition of $(H')^\ell$ is not unique, and by the assumption that $s \le \sqrt{\ell}$, the double summation makes sense.) We will, eventually, bound the Schmidt rank of each $Q_{i,\ell k}$.

To do that, we define a generating function that includes all the matching $f_{a_0,\dots,a_{s+1}}$'s:

$$P_{i,\ell k}(Z) = \sum_{\substack{a_i=k \\ \sum_{j\neq i} a_j = \ell-k}} f_{a_0,\dots,a_{s+1}} \prod_{j\neq i} Z_j^{a_j}.$$

This sum has $t = \binom{l-k+s}{s}$ terms as it is the same as the number of different sequences $(a_1, \dots a_{s+1})$ (w.l.o.g assume $i = 0$), with $a_1 + \ldots + a_s = \ell - k$. In this function, the variable Z_i is excluded, or we may consider it to be equal to 1. When the remaining variables are assigned definite values, $Z \in \mathbb{C}^{s+1}$, we obtain a linear combination of the operators $f_{a_0,\dots,a_{s+1}}$. (with each constant equals to $\prod_{j\neq i} Z_j^{a_j}$.)

The key observation is that such linear combinations have full rank because there cannot be more than t numbers of distinct $f_{a_0,\dots,a_{s+1}}$'s. Then in other words, there are t distinct values of $Z \in \mathcal{C}^{s+1}$ such that the corresponding $\{P_{i,\ell k}(Z)\}$ form a basis in the space of operators of the form $\sum c_{a_0,\dots,a_{s+1}} f_{a_0,\dots,a_{s+1}}$, where $c_{a_0,\dots,a_{s+1}} \in \mathbb{C}$ and the sum runs over the support of $P_{i,\ell k}$. In particular, $Q_{i,\ell k}$ is a linear combination of t operators of the form $P_{i,\ell k}(Z)$ with some definite Z's.

For a fixed Z, the operator $P_{i,\ell k}(Z)$ can be obtained as follows. We write $P_\ell(Z) = (A + H_i + B)^\ell$ where $A = \sum_{j<i} H_j Z_j$ and $B = \sum_{j>i} H_j Z_j$, and then collect the terms with H_i appearing exactly k times. since A and B commute, such terms have the form $A^{a_0} B^{b_0} H_i \cdots H_i A^{a_k} B^{b_k}$. The number of distinct terms like this is the same as the number of different sequences $(a_0, b_0, \dots, a_k, b_k)$, with $a_0 + b_0 + \ldots + a_k + b_k = \ell - k$. So there are $\binom{\ell-k+2(k+1)-1}{2(k+1)-1} = \binom{\ell+k+1}{2k+1}$

distinct terms like that.

The Schmidt rank of each term across cut i is at most d^{2k}, where d is the local dimension of particles. (H_i has Schmidt rank at most d^2 as with dimension d, there are d^2 possibilities of $L_i \otimes R_i$, and then k numbers of H_i will lead to Schmidt rank at most d^{2k}.) We can then write the Schmidt decomposition of the term as $\sum_{j=1}^{d^{2k}} C_j^{\mathrm{I}} \otimes D_j^{\mathrm{II\ \&\ III}}$, where I, II and III describes regions shown in Figure 2.3. Now we consider the middle cut. In this regards, we need to further Schmidt decompose $D_j^{\mathrm{II\ \&\ III}}$ as D_j acts on both region II and III. There are $|i - s/2|$ qubits in region II and $s/2$ qubits in region III, so the Schmidt rank of $D_j^{\mathrm{II\ \&\ III}}$ is at most $\left(d^{\min\{|i-s/2|, s/2\}}\right)^2 = d^{2|i-s/2|}$, where the first expression comes from Theorem 1.3 in [21]. Therefore the Schmidt rank across the middle cut is bounded by $d^{2k} \cdot (d^2)^{|i-s/2|} \leq d^s$.

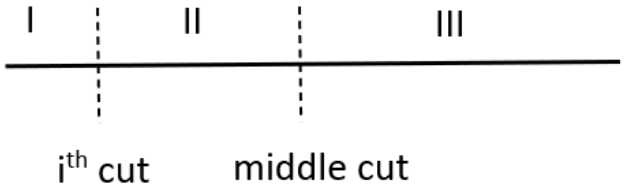

Figure 2.3: The Schmidt Rank of Each Term across the Middle Cut.

Also here, if we consider the Schmidt rank across an arbitrary cut, we just need to reconsider the number of qubits between cut i and the middle cut, but it will not have any impact asymptotically.

For each factor, given $k \leq \ell/s$ and $s \leq \sqrt{\ell}$, we calculate the asymptotic bound,

$$\begin{aligned}\binom{\ell - k + s}{s} &= \text{the number of different sequences } (a_1, \ldots a_{s+1}) \text{ with } a_1 + \ldots + a_s = \ell - k \\ &\leq \text{the number of sequences } (a_1, \ldots a_{s+1}) \text{ with each } a_j \leq l \\ &\leq \ell^{s+1} \\ &\leq \ell^{\mathcal{O}(s)},\end{aligned}$$

and then

$$\begin{aligned}\binom{\ell + k + 1}{2k + 1} &= \binom{\ell - k + (2k+1)}{2k+1} \\ &\leq \ell^{\mathcal{O}(2k+1)} \\ &= \ell^{\mathcal{O}(k)} \\ &\leq \ell^{\mathcal{O}(\ell/s)}.\end{aligned}$$

Combining all factors, we find that

$$\text{Schmidt rank}\,(Q_{i,\ell k}) \leq \binom{\ell-k+s}{s}\binom{\ell+k}{2k+1}d^{2k+s} \leq \ell^{\mathcal{O}(s)}\ell^{\mathcal{O}(\ell/s)}d^{2\ell/s+s} \leq (d\ell)^{\mathcal{O}(\ell/s)}.$$

Then $(H')^\ell = \sum_{i=1}^{s}\sum_{k=0}^{\ell/s} Q_{i,\ell k} \leq (d\ell)^{\mathcal{O}(\ell/s)}$ as the summation over i and k will not influence the bound in this asymptotic form. It follows that the Schmidt rank of $K = C_\ell(H')$, $D \leq (d\ell)^{\mathcal{O}(\ell/s)}$ as $(H')^\ell$ is the term with highest powers and then the remaining terms will not increase the bound in the asymptotic form.

End of proof.

Then together this bound with our previously obtained expression $\Delta = 4e^{-4\ell\sqrt{\epsilon/\|H'\|}}$ (recall that for truncated Hamiltonian H', we have $\|H'\| \leq s + 2t$), we decide to choose $\ell = \mathcal{O}(s^2)$ and $s = \mathcal{O}((\log^2 d)/\epsilon)$, so that with large enough constants, we can force

$$D \cdot \Delta = (d\ell)^{\mathcal{O}(\ell/s)} \cdot 4e^{-4\ell\sqrt{\epsilon/\|H'\|}} \leq \frac{1}{2}.$$

(See [6] Theorem 4.3 for detailed discussions about the choice of parameters.)
Therefore, by Theorem 2.3.3, we can conclude that there exists an area law for 1D gapped (frustration-free) systems.

2.4 Discussion of Frustrated Hamiltonian

The difference in the frustrated case is that when we consider the truncated Hamiltonian $H'(t) = H_L^{\leq t} + H_1 + \ldots + H_s + H_R^{\leq t}$ (defined in subsection 2.3.5), it no longer has the same ground state $|\Gamma\rangle$. But the structure of the samll eigenvectors and eigenvalues of $H'(t)$ should approach those of H as t grows.

The main idea for frustrated case is to use a well chosen sequence $t_0, t_1, \ldots$ to guide the movement towards the ground state i.e. to use a sequence of states $|\psi_0\rangle, |\psi_1\rangle, \ldots$ that converge to $|\Gamma\rangle$, while carefully controlling the tradeoff between increase in entanglement rank (D) and increase in overlap (Δ) with $|\Gamma\rangle$. Unlike directly applying Lemma 2.3.4 to H' which may lead to D becoming a large function of t, we use the AGSP $K = C_\ell(H'(t_i))$ from Lemma 2.3.4 to move from state ψ_{i-1} to ψ_i, where ψ_i has overlap at least $1-\mu_i$ with $|\phi^{t_i}\rangle$, the ground state of $H'(t_i)$.

A detailed explanation and arguments are in Section 6 of [6].

2.5 Discussion of Degenerate Ground States

In the above proof, we assume a 1D ground space of the quantum system which means H has a unique ground state. In [18], an area law is proved for the Renyi entanglement entropy of degenerate ground states in 1D gapped system, and an area law for the Renyi entanglement entropy implies that for von Neumann entropy.

Steps of the proof are similar to the method presented above by using AGSP to bound the increase of Schmidt ranks and then proving an efficient construction of AGSP will imply an area law. [18] first constructs a family of AGSP with nearly degenerate ground states with some perturbation theory involved also using Chebyshev polynomial. Then it constructs a sequence of approximations to basis vectors of the ground state space (here it requires new ideas to keep track of such a set of basis vectors) to prove the area law. The construction presented here is claimed to be more efficient than the approach (Corollary 2.4 and Section 6.2) in [6], resulting in an area law for the Renyi entanglement entropy and then it follows for von Neumann entropy.

Detailed proofs and explanation are in [18]. Note that the degeneracy we discuss here is constant-fold degeneracy, i.e. ground space should be of constant dimension even if not 1D. It is still unknown whether area laws hold when the ground space is of dimension polynomial in n [18].

Chapter 3

Introduction to Quantum Models

3.1 XXZ Model

The Heisenberg Model is a statistical mechanical model used in the study of critical points and phase transitions of magnetic systems, in which the spins of the magnetic systems are treated quantum mechanically. In a quantum system, we usually classify a certain model by a Hamiltonian, which is the sum of kinetic energies of all particles (qubits), plus the potential energy of the particles associated with the system.

Quantum mechanically, nearest-neighbors will have the lowest energy when they are aligned because of the dominant coupling between two dipoles. So we assume magnetic interactions only happen between neighbouring dipoles. Under this assumption, we have the Hamiltonian for a 1D non periodic lattice (chain) with n qubits:

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{n-1} \left(J_x X_i X_{i+1} + J_y Y_i Y_{i+1} + J_z Z_i Z_{i+1} + h Z_i\right),$$

where $Z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $X_i = I^{\otimes i-1} \otimes X \otimes I^{\otimes n-i}$ and similar for Y_i and Z_i (I is the 2×2 identity matrix). X, Y and Z are Pauli spin-$\frac{1}{2}$ matrices, which are quantum operators acting on the tensor product $(\mathbb{C}^2)^{\otimes n}$. J_x, J_y and J_z are three coupling constants, and h represents the external magnetic field, with non periodic boundary conditions here.

In the case that $J_x = J_y \neq J_z$, the model is called the Heisenberg XXZ model. We rewrite the Hamiltonian construction:

$$H = J\sum_i X_i X_{i+1} + Y_i Y_{i+1} + \Delta Z_i Z_{i+1} + h Z_i,$$

where J is the coupling constant for 1D model consisting of n qubit, Δ is a parameter that

controls the anisotropy in the z direction. Note that if $\Delta = 0$, it recovers XX model and if $\Delta = 1$, it recovers XXX model.

For our interest, we set $h = 0$ so that there are no external magnetic fields, and the exact solution is given by the Bethe Ansatz technique [7]. We can choose J arbitrarily since we only focus on normalized states and J will have no influence. Only XXZ model with $|\Delta| > 1$ is gapped, i.e. there is a gap between the ground state and the first excited state. We discuss $|\Delta| \leq 1$ in the next paragraph, and for $\Delta \longrightarrow \pm\infty$, we will recover classical Ising model, which is also not gapped. There is no specific argument about at which Δ the system is no longer gapped. We choose to focus on $1 < \Delta < 99$ in this paper, which should satisfy an area law. We investigate this property in Section 5.1

Also note that different Δs give different ground state structures. For $\Delta < -1$ the system is ferromagnetic and the exact ground state has all atoms aligned in the z-direction, i.e. $|\Gamma\rangle = |0 \dots 0\rangle$ or $|\Gamma\rangle = |1 \dots 1\rangle$. For $-1 < \Delta < 1$ the ground state is co-planar, with zero expectation value for $\langle S_z \rangle$, i.e. the ground state has almost equal number of $|0\rangle$s and $|1\rangle$s. In the Ising limit $\Delta \longrightarrow \infty$, the ground state would be the Néel state, with alternate $|0\rangle$s and $|1\rangle$s [23].

In the thesis, I mainly investigate on $\Delta \geq 0$, especially $1 < \Delta < 99$. So I choose to assume that the ground state would be in the form of almost equal number of $|0\rangle$s and $|1\rangle$s, i.e. the total spin is minimized. This is because for the range of Δs I pick, they are closer to 1 compared to ∞. Also, even if these ground state structures gradually approach ground state structures in the Ising limit, it does not make much effect because later cases are included in the previous cases. For example, for 4 qubits with $-1 < \Delta < 1$, a ground state can be written only with $\{|0011\rangle, |0101\rangle, |0110\rangle, |1001\rangle, |1010\rangle, |1100\rangle\}$. But with $\Delta \longrightarrow \infty$, a ground state can be written only with $\{|0101\rangle, |1010\rangle\}$. In this way, if we choose the previous basis, ground states lying into the later case can also be represented with coefficients 0 for useless vectors in the basis.

We also make a few remarks about the entanglement entropy of the ground state of XXZ model with $-1 < \Delta \leq 1$, where the system is in the gapless critical XY phase. The scaling law of entanglement entropy for finite sizes is

$$S_A(l, L) = \frac{c + \bar{c}}{6} \log \left[\frac{L}{\pi} \sin \left(\frac{\pi l}{L} \right) \right] + k,$$

for a subsystem of size l and total size L. c and $\bar{c}$ in the equation are parameters related to conformal field theory [9]. $\Delta = -1$ is proved to cause a singularity in the entanglement entropy [12] [13]. As for $\Delta \longrightarrow -1^+$, it is proved that the entanglement entropy scales logarithmically with L, the number of qubits [24] [10].

3.2 XXZ-Variant Model

As the Hamiltonian for normal XXZ model is not frustration free and possible AGSP in the form of $I - \frac{H}{\|H\|}$ is proposed in [15], we would like to see how frustration free Hamiltonian acts under such possible AGSP. [8] discusses the construction of a frustration free gapped Hamiltonian: Consider a chain of n qubits with open boundary conditions and define a Hamiltonian

$$H_n(\psi) = \sum_{i=1}^{n-1} |\psi\rangle \langle\psi|_{i,i+1} .$$

Here each term is a rank-1 projector onto ψ applied to a consecutive pair of qubits.

For a special kind of XXZ model - the ferromagnetic XXZ chain with kink boundary conditions, which we call it XXZ-Variant Model here, we have

$$|\psi\rangle = \frac{1}{\sqrt{1+q^2}} |01\rangle - q\,|10\rangle ,$$

and when $q \neq 1$, the corresponding system is gapped which is proved in [15].

However, the ground-state space of the Hamiltonian is not of constant dimension. Instead, it has ground state degeneracy $n+1$ which is a polynomial in n. As we discussed in Section 2.5, an area law is not yet proven to exist under this case and so we do not know how its entanglement entropy grows with increasing number of qubits theoretically. We will still investigate this relationship experimentally in Section 5.2, but we will stop there instead of continuing to investigate its corresponding AGSP.

3.3 AKLT Model

Unlike the XXZ model describing a chain of qubits (spin-1/2 particles), the AKLT model focuses more on a spin-1 system. In particular, this model is interested in constructing a one-dimensional state with a valence bond between every pair of sites. This leads to two spin-1/2 particles for every site, and the result will be a spin-1 chain.

As described in [2], to find a Hamiltonian for which the chain described above is the ground state, we choose the Hamiltonian to be a sum of projection operators onto spin 2 for each neighboring pair (denoted as $P^{S=2}_{i,i+1}$). This is because the a valence bond between adjacent spin-1/2 particles implies that the total spin of each pair site cannot be 2. (Two of the spin-1/2 particles will form a singlet. For short chains, the edge states mix into either a singlet or a triplet giving either a unique ground state (closed chain) or a three-fold multiplet of

ground states.) Here is the Hamiltonian:

$$\begin{aligned} H &= \sum_i P_{i,i+1}^{S=2} \\ &= \sum_i \left[\frac{1}{2} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{6} \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} \right)^2 + \frac{1}{3} \right], \end{aligned}$$

where $\mathbf{S} = (S^1, S^2, S^3)$ is the vector of standard spin-1 matrices.

It is also claimed in [2] that

1. The ground-state energy of this Hamiltonian is zero.
2. In the infinite-volume limit (n goes to infinity) there is always a unique ground state.
3. There is a non-vanishing gap in the spectrum above the ground state. (This is also discussed and investigated rigrously in [14] which is to investigation on the spectral gap using Tensor Network.)

Since the ground state will vanish with n goes to infinity, we can conclude that the ground-state degeneracy will not be of polynomials of n and so there exists an area law for AKLT model. But since the Hilbert space grows with 3^n, where n is the number of qubits, by the limitation of computation power and understanding of spin-1 model, we will just investigate its entropy entanglement growth.

Chapter 4

Numerical Techniques to Study Physical Models

4.1 Standard Construction

To study the low-energy physics of a certain model, it is common to start from its Hamiltonian which describes and classifies a certain system. Then from this Hamiltonian, we can get information from its eigensystem, which is always the focus of interest as it is frame invariant.

To study the area law on certain model, we focus on the ground state. Then through Schmidt decompostion, we find ground state's Schmidt coefficients and entanglement entropy, as defined in Chapter 1. The formal steps are defined below:

Input : Parameters needed to construct the Hamiltonian.

1. Compute Hamiltonian matrix H of a certain model based on its definition.
2. Find the ground state v of the Hamiltonian H.
3. Find the Schmidt decomposition v and record its Schmidt coefficients $\{\lambda_i\}$.
4. Calculate the entanglement entropy of the model across certain cut, according to $\{\lambda_i\}$.

Output : Schmidt Coefficients / Entanglement Entropy

Algorithm 1: Standard Algorithm for Model Construction

Take the XXZ Model as an example, in step 1, we compute its Hamiltonian by

$$H = J \sum_i X_i X_{i+1} + Y_i Y_{i+1} + \Delta Z_i Z_{i+1},$$

where J is the coupling constant for 1D model consisting of n qubit, Δ is a parameter that

controls the anisotropy in the z direction, and X, Y, Z are Pauli matrices defined before.

4.2 Quicker Construction based on Hamming Weights

When the number of qubits n grows, the dimension $2^n \times 2^n$ of H grows very fast, which makes matrix multiplication and Schmidt decomposition very slow. But by the intuition that relatively equal number of ups and downs balance each other, giving the lowest energy, we know that the ground state is only associated with states of almost the same number of 0s and 1s. Therefore, we design an algorithm to construct the Hamiltonian only associated with these states. Formal steps are presented below:

Input : Parameters needed to construct the Hamiltonian.

1. Compute the Hamiltonian matrix $\widetilde{H}$ of a certain model based on its definition, but with basis $\widetilde{b}$ consisting of almost equal numbers of 0s and 1s
2. Find the ground state $\tilde{v}$ of the Hamiltonian $\widetilde{H}$.
3. Refill the ground state $\tilde{v}$ with 0 under original basis b (dimension $= 2^n$), call the new one v. (Detailed explanations are given below by an example.)
4. Find the Schmidt coefficients $\{\lambda_i\}$ of v.
5. Calculate the entanglement entropy of XXZ model across certain cut, according to $\{\lambda_i\}$.

Output : Schmidt Coefficients, Entanglement Entropy

Algorithm 2: Quicker Algorithm for Model Construction

Note that $\widetilde{H} = PHP^T$, where P is a change of basis matrix, such that

$$P_{ij} = \left\langle \widetilde{b_i} \,\middle|\, b_j \right\rangle = \left(\widetilde{b_i}\right)^T \cdot b_j.$$

Also, the size of $\widetilde{H}$ is either $\binom{n}{n/2} \times \binom{n}{n/2}$ (even n) or $2\binom{n}{n/2} \times 2\binom{n}{n/2}$ (odd n). Schmidt coefficients generated by Algorithm 2 gives exact Schmidt coefficients by the validity of the algorithm which we will argue later.

We mainly implement this algorithm for XXZ model and we show how to generate the ground state Hamiltonian $\widetilde{H}$ for XXZ model through the following procedure:

Input : n,J and Δ.

1. For any basis element $p \in \widetilde{b}$, we write it in bra-ket notation $|p\rangle = |p_1 p_2 \dots p_n\rangle$.
2. Then we count the number of pairs 00 and 11 in s and call it d, i.e. the number of i's such that $p_i = p_{i+1}$. It automatically follows that the number of pairs 01 and 10 is $n-1-d$.
3. For every pair 01 or 10, we switch its position which leads to a new state q_i. In other words, for every $p_j \neq p_{j+1}$, we generate $|q_j\rangle = |p_1 \dots p_{j+1} p_j \dots p_n\rangle$. (Note that we have $n-1-d$ $|q_j\rangle$'s.)
4. We then compute $|p'\rangle = \Delta(d-(n-d-1))\,|p\rangle + 2\sum_j |q_j\rangle$ for all $p \in \widetilde{b}$. We relabel $|p\rangle$ as $\left|\widetilde{b_i}\right\rangle$ and calculate $\left|\widetilde{b'_i}\right\rangle = |p'\rangle$ for all $\widetilde{b_i}$ using the formula.
5. Then we come up with $\widetilde{H}_{ij} = \left\langle \widetilde{b_i} \middle| \widetilde{b'_j} \right\rangle$.

Output : Schmidt Coefficients / Entanglement Entropy

Algorithm 3: Quicker Algorithm for XXZ Model Construction

As for the second refill step in algorithm 3, we do it by expanding $\widetilde{v} = \sum_i \widetilde{c_i}\widetilde{b_i}$ to $v = \sum_i c_i b_i$, in the way that if $b_i = \widetilde{b_i}$ in the bra-ket notation, we let $c_i = \widetilde{c_i}$ and otherwise we let $c_i = 0$.

Still taking XXZ Model as an example, we choose the number of qubits $n = 3$. Basis states with almost equal numbers of 0s and 1s in string forms are $|001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle$ and they form a basis $\widetilde{b}$. We then construct the Hamiltonian with basis $\widetilde{b}$, following above algorithm.

state p or $\widetilde{b_i}$	d	$n-1-d$	$\{q_j\}$	$\widetilde{b'_i}$
$\|001\rangle$	1	1	$\|010\rangle$	$2\,\|010\rangle + 0\,\|001\rangle$
$\|010\rangle$	0	2	$\|100\rangle$, $\|001\rangle$	$2\,\|100\rangle$+2$\|001\rangle + 2\Delta\,\|010\rangle$
$\|011\rangle$	1	1	$\|101\rangle$	$2\,\|101\rangle + 0\,\|011\rangle$
$\|100\rangle$	1	1	$\|010\rangle$	$2\,\|010\rangle + 0\,\|100\rangle$
$\|101\rangle$	0	2	$\|011\rangle$, $\|110\rangle$	$2\,\|011\rangle$+2$\|110\rangle + 2\Delta\,\|101\rangle$
$\|110\rangle$	1	1	$\|101\rangle$	$2\,\|101\rangle + 0\,\|110\rangle$

Table 4.1: Parameters for Implementation of Algorithm 3

It follows that

$$\widetilde{H} = \begin{pmatrix} \langle \widetilde{b}_1 | \widetilde{b}'_1 \rangle & \langle \widetilde{b}_1 | \widetilde{b}'_2 \rangle & \langle \widetilde{b}_1 | \widetilde{b}'_3 \rangle & \langle \widetilde{b}_1 | \widetilde{b}'_4 \rangle & \langle \widetilde{b}_1 | \widetilde{b}'_5 \rangle & \langle \widetilde{b}_1 | \widetilde{b}'_6 \rangle \\ \langle \widetilde{b}_2 | \widetilde{b}'_1 \rangle & \langle \widetilde{b}_2 | \widetilde{b}'_2 \rangle & \langle \widetilde{b}_2 | \widetilde{b}'_3 \rangle & \langle \widetilde{b}_2 | \widetilde{b}'_4 \rangle & \langle \widetilde{b}_2 | \widetilde{b}'_5 \rangle & \langle \widetilde{b}_2 | \widetilde{b}'_6 \rangle \\ \langle \widetilde{b}_3 | \widetilde{b}'_1 \rangle & \langle \widetilde{b}_3 | \widetilde{b}'_2 \rangle & \langle \widetilde{b}_3 | \widetilde{b}'_3 \rangle & \langle \widetilde{b}_3 | \widetilde{b}'_4 \rangle & \langle \widetilde{b}_3 | \widetilde{b}'_5 \rangle & \langle \widetilde{b}_3 | \widetilde{b}'_6 \rangle \\ \langle \widetilde{b}_4 | \widetilde{b}'_1 \rangle & \langle \widetilde{b}_4 | \widetilde{b}'_2 \rangle & \langle \widetilde{b}_4 | \widetilde{b}'_3 \rangle & \langle \widetilde{b}_4 | \widetilde{b}'_4 \rangle & \langle \widetilde{b}_4 | \widetilde{b}'_5 \rangle & \langle \widetilde{b}_4 | \widetilde{b}'_6 \rangle \\ \langle \widetilde{b}_5 | \widetilde{b}'_1 \rangle & \langle \widetilde{b}_5 | \widetilde{b}'_2 \rangle & \langle \widetilde{b}_5 | \widetilde{b}'_3 \rangle & \langle \widetilde{b}_5 | \widetilde{b}'_4 \rangle & \langle \widetilde{b}_5 | \widetilde{b}'_5 \rangle & \langle \widetilde{b}_5 | \widetilde{b}'_6 \rangle \\ \langle \widetilde{b}_6 | \widetilde{b}'_1 \rangle & \langle \widetilde{b}_6 | \widetilde{b}'_2 \rangle & \langle \widetilde{b}_6 | \widetilde{b}'_3 \rangle & \langle \widetilde{b}_6 | \widetilde{b}'_4 \rangle & \langle \widetilde{b}_6 | \widetilde{b}'_5 \rangle & \langle \widetilde{b}_6 | \widetilde{b}'_6 \rangle \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 2 & 0 & 0 & 0 & 0 \\ 2 & 2 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 2 & 2 \\ 0 & 0 & 0 & 0 & 2 & 0 \end{pmatrix}.$$

We now argue the validity and accuracy of this quicker method. Firstly, we prove that ground state basis is preserved under $H = J\sum_i X_iX_{i+1} + Y_iY_{i+1} + \Delta Z_iZ_{i+1}$.

Proposition 4.2.1. *Ground state basis $\widetilde{b}$ is preserved under $H = J\sum_i X_iX_{i+1} + Y_iY_{i+1} + \Delta Z_iZ_{i+1}$.*

Proof. We first consider $(X_iX_{i+1} + Y_iY_{i+1})\,|xy\rangle_{i,i+1}$:

$$\begin{aligned} (X_iX_{i+1} + Y_iY_{i+1})\,|01\rangle_{i,i+1} &= |10\rangle + (-i)^2\,|10\rangle = 2\,|10\rangle \\ (X_iX_{i+1} + Y_iY_{i+1})\,|10\rangle_{i,i+1} &= |01\rangle + (-i)^2\,|01\rangle = 2\,|01\rangle \\ (X_iX_{i+1} + Y_iY_{i+1})\,|00\rangle_{i,i+1} &= |11\rangle + (-i)^2\,|11\rangle = 0 \\ (X_iX_{i+1} + Y_iY_{i+1})\,|11\rangle_{i,i+1} &= |00\rangle + (-i)^2\,|00\rangle = 0 \end{aligned}$$

It is easy to see that $(X_iX_{i+1} + Y_iY_{i+1})$ will not change Hamming weights of $|xy\rangle_{i,i+1}$. Then we consider Z_iZ_{i+1} on $|xy\rangle$. Because Z will only change the symbol of a state, i.e. $|xy\rangle$ will be changed to $(-1)^{x\oplus y}\,|xy\rangle$.

Since Hamming weight is not changed by H, the ground state basis $\widetilde{b}$ is preserved under H.

End of proof.

We then prove that $\widetilde{H}$ constructed in algorithm 3 is correct corresponding ground state matrix of H, i.e. $Hb_i = \widetilde{H}\widetilde{b_i}$, where $b_i = \widetilde{b_i}$ in the bra-ket notation, but different in the vector notation. For example, for $b_i = |001\rangle = \widetilde{b_i}$ in the bra-ket form, we have $b_i = (0\ 1\ 0\ 0\ 0\ 0\ 0\ 0)^T$ and $\widetilde{b_i} = (1\ 0\ 0\ 0\ 0\ 0)^T$ in the vector form.

Proposition 4.2.2. $Hb_i = \widetilde{H}\widetilde{b_i}$

Proof. In bra-ket notation, we have $Hb_i = H\widetilde{b_i}$ and by the construction of $\widetilde{H}$, we have $\widetilde{H}\widetilde{b_i} = \widetilde{b_i'}$. So it suffices to prove that $H\widetilde{b_i} = \widetilde{b_i'}$ in the bra-ket notation.

For convenience, we relabel $\widetilde{b_i}$ as p again to avoid subscripts.

$$\begin{aligned}
H\left|\widetilde{p}\right\rangle &= \left(\sum_i X_iX_{i+1} + Y_iY_{i+1} + \Delta Z_iZ_{i+1}\right)|p_1 \dots p_n\rangle \\
&= \sum_i \left(\left(X_iX_{i+1} + Y_iY_{i+1}\right)|p_1 \dots p_n\rangle + \Delta Z_iZ_{i+1}|p_1 \dots p_n\rangle\right) \\
&= \sum_i \left(2\,|p_1 \dots \overline{p_i}\ \overline{p_{i+1}} \dots p_n\rangle + \Delta(-1)^{p_i \oplus p_{i+1}}|p_1 \dots p_n\rangle\right) \\
&= \sum_{i,\ \text{s.t.}\ p_i \neq p_{i+1}} \left(2\,|p_1 \dots p_{i+1}\ p_i \dots p_n\rangle + \Delta(-1)^{p_i \oplus p_{i+1}}|p_1 \dots p_n\rangle\right) \\
&= \left(\sum_{i,\ \text{s.t.}\ p_i \neq p_{i+1}} 2\,|p_1 \dots p_{i+1}\ p_i \dots p_n\rangle\right) + \Delta(d - (n-1-d))\,|p_1 \dots p_n\rangle \\
&= \left(\sum_j 2\,|q_j\rangle\right) + \Delta(d - (n-1-d))\,|p\rangle \\
&= |p'\rangle
\end{aligned}$$

where the third equality comes from the proof of Proposition 4.2.1. The forth equality comes from the fact that if $p_i = p_{i+1}$, then it will vanish under $X_iX_{i+1} + Y_iY_{i+1}$. So only $p_ip_{i-1} = 01$ or 10 will be left and it follows that $\overline{p_i}\ \overline{p_{i+1}} = p_{i+1}p_i$. The fifth equality comes from the fact that there are d number of pairs 00 and 11 such that $p_i \oplus p_{i+1} = 0$ and $n-1-d$ number of pairs 01 and 10 such that $p_i \oplus p_{i+1} = 1$.

End of proof.

4.3 Construction by Density Matrix Renormalization Group

4.3.1 Brief Introuction

The density matrix renormalization group (DMRG) we will introduce here is a numerical variational algorithm that attempt to find an approximate Hamiltonians of a quantum many-body system. It was first proposed White in 1992 [27] and it is one of the most efficient techniques for 1D systems.

The main problem of quantum system simulation is that the Hilbert space grows exponentially with number of qubits n, which touches the limitation of classical computational power very quickly. Even though compared to Algorithm 1, Algorithm 2 saves us a $\sqrt{2}$ factor since $\binom{n}{n/2} \approx \frac{2^n}{\sqrt{n}}$. As for DMRG, it is an iterative technique which aims to "collect" the most important information for a target state. DMRG scales polynomially with respect to the size of the active space, which can be determined by investigators. Detailed analysis on the complexity on DMRG can be found in [25].

DMRG's idea of increasing the system but not increasing the Hilbert space is typically based on two steps: The number of qubits n increases and consequentially the Hilbert space grows at the same time. Then the Hilbert space is truncated to its original size keeping the system size invariant. We now describe DMRG more detailedly with an example of 1D XXZ model below based on the reference [20].

4.3.2 Single Enlargement and Truncation in DMRG

We first describe how the single enlargement and truncation step works in DMRG theoretically and will give an example later to better explain this step.

The elementary unit in the step is a site with dimension D, i.e. a qubit for our interest. The step usually is given an input m, which is the number of states kept.

1. We start with a block $B(l, m)$, consisting of number of sites l where l is the minimum number of qubits such that $2^l > m$. We also have a Hamiltonian H_B associated with $B(l, m)$, with basis $\{|b_1\rangle, \ldots, |b_m\rangle\}$.

2. The block is enlarged by adding another site to it and they then form the enlarged block B^e with dimension $(m \times D) \times (m \times D)$. The basis now is $\{|b_k^e\rangle = |b_i\rangle \otimes |d_j\rangle\}$, where $\{|d_1\rangle, \ldots, |d_D\rangle\}$ is the basis of the new added site, and $k = (i-1)D + j$.

3. We now form the superblock Hamiltonian, which consists of two enlarged blocks connected to each other. The left enlarged block is the one we get in previous step and the right one is the reflected enlarged block. Then the target state (ground sate for our interest) of the superblock is computed and we expressed that in the form

$$|\Psi_0\rangle = \sum_{i=1}^{m\times D} \sum_{i=1}^{m'\times D} a_{ij} |b_i^e\rangle \otimes \left|b_j'^e\right\rangle, \tag{4.1}$$

   where the prime refers to the parameters associated the right enlarged block. For a infinite system, we usually have $M' = m$ while for a finite system, we have $m' = m$ or $m = n - m' + 1$.

4. We then use the ground states to form a density matrix with entries:

$$\rho_{ii'} = \sum_{i=1}^{m' \times D} a_{ij} a^*_{i'j}. \tag{4.2}$$

We denote the eigenstates of ρ as $|u_\alpha\rangle$ $(\alpha = 1, \ldots, m \times D)$ and eigenvalues w_α. Note that these eigenvalues represent the probability of the system being in the state $|u_\alpha\rangle$ given that the universe is in the state $|\Psi_0\rangle$. Since we want to truncate H_e to only stay with several important states and neglect all others to keep the Hilbert space constant (size m), we order the $|u_\alpha\rangle$ by their eigenvalues in a decreasing order and only use the first m eigenvectors. We now form the transformation matrix O with size $m \times (m \times D)$ with these selected good eigenvectors.

5. We now construct the truncated Hamiltonian for the enlarged block, which then will be denoted as $B(l+1, m)$:

$$H_{B(l+1,m)} = O H_e O^\dagger. \tag{4.3}$$

Note that besides Hamiltonians being stored and updated during the process, we also need to keep track of operators representing the sites at the border of the block. These operators mostly give instruction on the interaction among blocks and sites. They also need to be enlarged when the block is enlarged, and truncated when the block Hamiltonian is truncated. We now give a detailed example to show how all the procedures work.

Given a 1D XXZ model with n qubits without external field, and we pick $m = 2$ so that the size of the approximated Hamiltonian should be limited to 2×2. Here is how single enlargement and truncation procedure works for such model.

1. We start from a block $B(1, 2)$ of a single site. Note that the possible states of the single site are $|b_1\rangle = |0\rangle$ and $|b_1\rangle = |1\rangle$. For one isolated site without external fields, the Hamiltonian H_B associated is a 0 matrix. We have operators associated as $S^x_b = X$, $S^y_b = Y$ and $S^z_b = Z$.

2. To build the enlarged system, another site is added with the same basis: $|d_1\rangle = |0\rangle$ and $|d_1\rangle = |1\rangle$. Then the basis of the enlarged block is (e stands for enlarged)

$$\begin{aligned} |b^e_1\rangle &= |00\rangle \\ |b^e_2\rangle &= |01\rangle \\ |b^e_3\rangle &= |10\rangle \\ |b^e_4\rangle &= |11\rangle \end{aligned}.$$

Now we have block $B(2, 4)$ instead of the original $B(1, 2)$. The Hamiltonian H_e for $B(2, 4)$ is no longer a 0 matrix and it should describe the interactions between two

sites (qubits) in $B(2,4)$ based the definition of Hamiltonian for XXZ model:

$$\begin{aligned}
H_e &= H_B \otimes I_d + H \\
&= H_B \otimes I_d - \frac{J}{2}\left(S_b^x \otimes S_d^x + S_b^y \otimes S_d^y + \Delta S_b^z \otimes S_d^z\right) \\
&= H_B \otimes I_d - \frac{J}{2}\left(X_b \otimes X_d + Y_b \otimes Y_d + \Delta Z_b \otimes Z_d\right) \\
&= \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
&- \frac{J}{2}\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\right] \\
&- \frac{J\Delta}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
&= -\frac{J}{2}\begin{pmatrix} \Delta & 0 & 0 & 0 \\ 0 & -\Delta & 2 & 0 \\ 0 & 2 & -\Delta & 0 \\ 0 & 0 & 0 & \Delta \end{pmatrix}
\end{aligned}$$

We also need to update our operators S_b^x, S_b^y, S_b^z as

$$\left(S_r^x\right)_e = I_b \otimes S_d^x = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

and similarly for $\left(S_r^y\right)_e$ and $\left(S_r^z\right)_e$.

3. We now construct a superblock by taking the enlarged block as the left block and connecting it to another enlarged block on the right. The right enlarged block is the same as the left block, only spatially reflected, which means that the qubit last added to the left block is connected to itself in the right block. The basis for this superblock

is given by:

$$\begin{pmatrix} |b_1^e\rangle \\ |b_2^e\rangle \\ |b_3^e\rangle \\ |b_4^e\rangle \end{pmatrix} \otimes \begin{pmatrix} |b_1'^e\rangle \\ |b_2'^e\rangle \\ |b_3'^e\rangle \\ |b_4'^e\rangle \end{pmatrix} = \begin{pmatrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{pmatrix} \otimes \begin{pmatrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{pmatrix} = \begin{pmatrix} |0000\rangle \\ |0001\rangle \\ |0010\rangle \\ |0011\rangle \\ |0100\rangle \\ |0101\rangle \\ |0110\rangle \\ |0111\rangle \\ |1000\rangle \\ |1001\rangle \\ |1010\rangle \\ |1011\rangle \\ |1100\rangle \\ |1110\rangle \\ |1111\rangle \end{pmatrix} = \begin{pmatrix} |b_1^s\rangle \\ |b_2^s\rangle \\ |b_3^s\rangle \\ |b_4^s\rangle \\ |b_5^s\rangle \\ |b_6^s\rangle \\ |b_7^s\rangle \\ |b_8^s\rangle \\ |b_9^s\rangle \\ |b_{10}^s\rangle \\ |b_{11}^s\rangle \\ |b_{12}^s\rangle \\ |b_{13}^s\rangle \\ |b_{14}^s\rangle \\ |b_{15}^s\rangle \\ |b_{16}^s\rangle \end{pmatrix}.$$

Our target state is the ground state and so we only focus on 6 states with same number of 0s and 1 which belong to the ground space (similar to the idea in Algorithm 2):

$$\begin{aligned} \left|b_1^{s(0)}\right\rangle &\equiv |b_4^s\rangle = |b_1^e\rangle \otimes |b_4' e\rangle \\ \left|b_2^{s(0)}\right\rangle &\equiv |b_6^s\rangle = |b_2^e\rangle \otimes |b_2' e\rangle \\ \left|b_3^{s(0)}\right\rangle &\equiv |b_7^s\rangle = |b_2^e\rangle \otimes |b_3' e\rangle \\ \left|b_4^{s(0)}\right\rangle &\equiv |b_{10}^s\rangle = |b_3^e\rangle \otimes |b_2' e\rangle \\ \left|b_5^{s(0)}\right\rangle &\equiv |b_{11}^s\rangle = |b_3^e\rangle \otimes |b_3' e\rangle \\ \left|b_6^{s(0)}\right\rangle &\equiv |b_{13}^s\rangle = |b_4^e\rangle \otimes |b_1' e\rangle \end{aligned}$$

The Hamiltonian of the superblock consists of three parts: the left enlarged block, the right enlarged block (i.e. the reflected left enlarged block) and the connecting interactions between these two blocks:

$$H_s = H_e \otimes I_e' + I_e \otimes H_e' - \frac{J}{2}\left((S_r^x)_e \otimes (S_r^x)_e' + (S_r^y)_e \otimes (S_r^y)_e' + \Delta\,(S_r^z)_e \otimes (S_z^x)_e'\right),$$

where the prime refers to the operators on the right enlarged block. We calculated this

H_s in the basis $\left|b_i^{s(0)}\right\rangle$:

$$-\frac{J}{2}\begin{pmatrix} \Delta & 0 & 2 & 0 & 0 & 0 \\ 0 & -\Delta & 2 & 2 & 0 & 0 \\ 2 & 2 & -3\Delta & 0 & 2 & 0 \\ 0 & 2 & 0 & -3\Delta & 2 & 2 \\ 0 & 0 & 2 & 2 & -\Delta & 0 \\ 0 & 0 & 0 & 2 & 0 & \Delta \end{pmatrix}.$$

If we take $J = -1/2$ and $\Delta = 1$, then the ground state energy of H_s^0 is $E_0 = 1/4(3 + 2\sqrt{3})$ and the ground state eigenvector is

$$|\psi_0\rangle = \begin{pmatrix} 1 \\ 1+\sqrt{3} \\ -2-\sqrt{3} \\ -2-\sqrt{3} \\ 1+\sqrt{3} \\ 1 \end{pmatrix} = \begin{pmatrix} a_{14} \\ a_{22} \\ a_{23} \\ a_{32} \\ a_{33} \\ a_{41} \end{pmatrix},$$

where the second equality comes from Equation 4.1 the correspondence basis $\left\{\left|b_i^{s(0)}\right\rangle\right\}$.

4. We now construct the density matrix using Equation 4.2

$$\rho = (a_{ij}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & (1+\sqrt{3})^2 + (-2-\sqrt{3})^2 & 2(1+\sqrt{3})(-2-\sqrt{3}) & 0 \\ 0 & 2(1+\sqrt{3})(-2-\sqrt{3}) & (1+\sqrt{3})^2 + (-2-\sqrt{3})^2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 11+6\sqrt{3} & -2(5+3\sqrt{3}) & 0 \\ 0 & -2(5+3\sqrt{3}) & 11+6\sqrt{3} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

We then calculate eigenvalues and eigenvectors of ρ to do the truncation step. Since we pick $m = 2$, we only pick two eigenvectors that correspond to largest two eigenvalues to construct the transformation matrix in Equation 4.3, which is

$$O = \begin{pmatrix} 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

5. This is the final step in this first procedure. We get the truncated Hamiltonian with

dimension $m \times m$ we will use in the iterative step for the enlarged bock:

$$H_{B(2,2)} = OH_eO^\dagger = \frac{1}{4}\begin{pmatrix} -3 & 0 \\ 0 & 1 \end{pmatrix}.$$

We also get the truncated operators using this transformation matrix too:

$$S_r^x = OS_r^xO^\dagger,$$

and similar for S_r^y and S_r^z.

4.3.3 The Infinite and Finite System DMRG

Given the single enlargement and truncation step in DMRG, the rest of DMRG is mostly about iterations. Here is the Inifite System DMRG:

1. Grow the chain normally to a size l in which its Hilbert space dimension is just larger than m, the number of states to be kept. ($m < 2^l$) We treat this as our first enlarged block.

2. Implement procedures in Section 4.3.2 to enlarge the left block size to $l + 1$ using the single step described in previous section: Form the superblock, calculate the density matrix and using transformation matrix to truncate the enlarged block. This truncated left enlarged block then will be used as the block for the next iteration.

3. Continue with step 2 until convergence is reached.

The Finite System DMRG is similar to the infinite one. The difference is that in the infinite case the right enlarged block used in the construction of the superblock is the same size as the left enlarged block. But in the finite case, the right enlarged block always complements the left one to the total number of qubits n and thus becomes shorter. We deal with the finite case by sweeping over the system again when the right block has only 1 qubit and so this again and again until convergence is achieved. Detailed explanation about the Infinite and Finite System DMRG are explained in [20]. Code for the implementation can be found on simple-dmrg.

Using DMRG, we will not get Hamiltonian scaling with $\mathcal{O}(2^n)$ which is the main problem in quantum simulation. After we get the approximate Hamiltonian with dimension $m \times m$, we can get the ground state and get Schmidt coefficients associated to calculate approximated entanglement entropy. We can set m small to compute approximate entropy very quickly, which would be very beneficial for the investigation of the area law.

Chapter 5

Area Law on Quantum Models

5.1 XXZ Model

5.1.1 Entropy Entanglement vs. Position of the Cut

We investigated how the position of the cut i influences the entanglement entropy. Theoretically it should not be significantly influence the entropy very much as otherwise we cannot prove the area law only for the middle cut. So for the investigation below, we expect that the entropy does not change when we vary cut i. Note that for an odd number of qubits, there are two ground states because intuitively for n qubits, the ground space can be formed by $(n+1)/2$ 0s and $(n-1)/2$ 1s or $(n-1)/2$ 0s and $(n+1)/2$ 1s. And we just arbitrarily choose one to evaluate its entanglement entropy, which any of then would follow an area law as described Section 2.5 and [18]. We set $J = 1$ (as it does not matter what the value of J is since we only consider normalized state) and here are the results with dashed lines represent odd # qubits and others represent even # qubits.

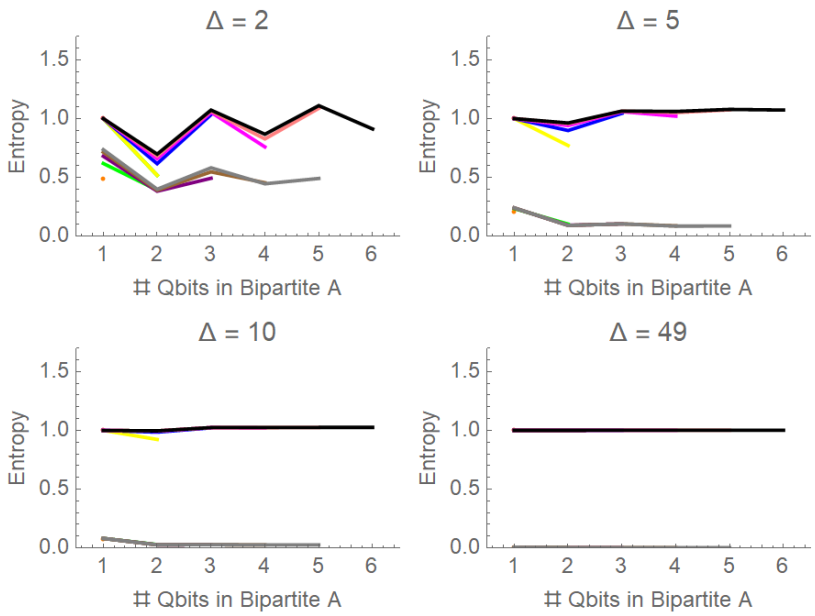

Figure 5.1: Entropy Entanglement vs. Position of the Cut for XXZ Model

We choose $\Delta = 2, 5, 10, 49$ for investigation here and for readers who are interested in seeing more, code is provided is Appendix B. It is clearly shown that independent of cut i, entropy is nearly stable and bounded by certain constant. With Δ gets larger, the stability is clearer, such that entropy stays around 1 and 0 for even and odd number of qubits respectively.

So we can conclude that XXZ model's entanglement entropy appears to follow area law independent of which cut we choose to separate the system.

5.1.2 Entropy Entanglement vs. Number of Qubits

Here we investigate the relationship between entanglement entropy and number of qubits n. Theoretically as mentioned before, since when $|\Delta| > 1$, XXZ model is a gapped system and so its 1D version should follow an area law. In the following experiment, we set still $J = 1$ and let cut i be the middle cut.

We expect to see that with $1 < \Delta < 99$ (assuming that $\Delta > 99$ to be large enough for XXZ model to approach the classical Ising model), entropy is always bounded by some constant as n increases. However, by the limitation of the computation power, we can only calculate up to $n = 14$. So here we expect to see entanglement entropy does not increase much so that we can see that the entropy appears to be bounded by a constant. Results generated by Algorithm 3 are in Figure 5.2 .

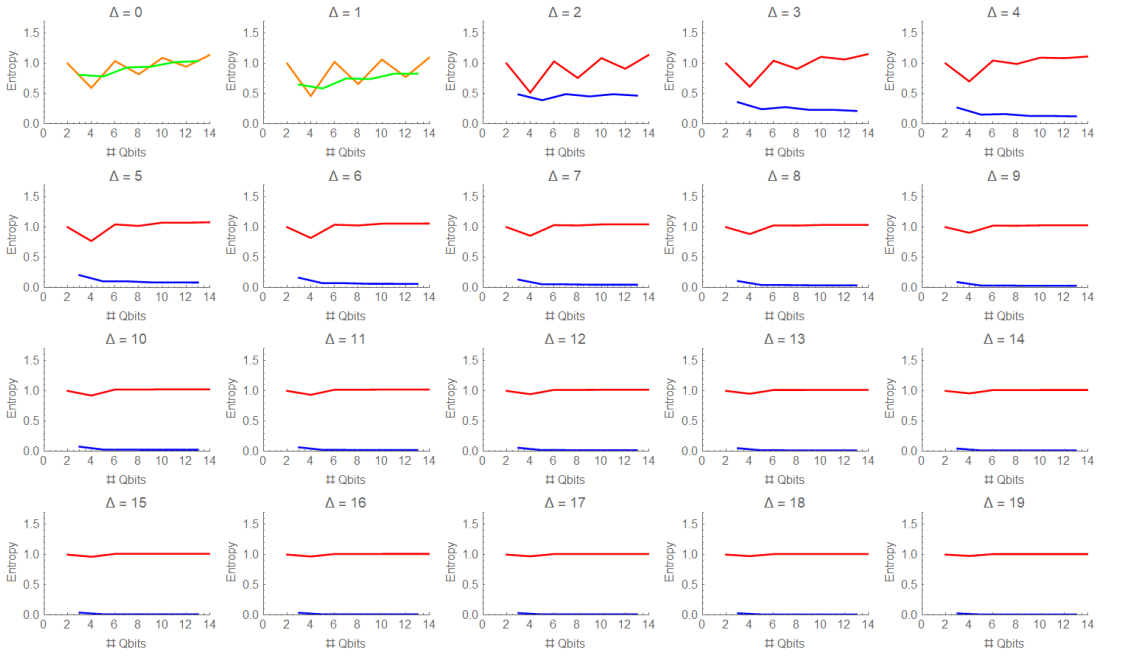

Figure 5.2: Entropy Entanglement vs. Number of Qubits for XXZ Model with $1 < \Delta < 99$

For $1 < \Delta < 99$, it is clear that entropy is very different for odd number of qubits and even number of qubits. For odd number of qubits, the entanglement entropy is closer to 0, especially when $\Delta \geq 3$, while the entropy is varying around 1. But for both of them, there is no significant increasing trend in the entanglement growth, so we can vaguely conclude that the entropy is bounded by $\mathcal{O}(1)$, which follows the theory.

With $|\Delta| \leq 1$, it is more obvious that entropy seems to follow a period trend with period = 4 and is slightly increasing (the increase is more obvious than that of larger Δ's). The result slightly reflects the logarithmic increase trend described in Section 3.1.

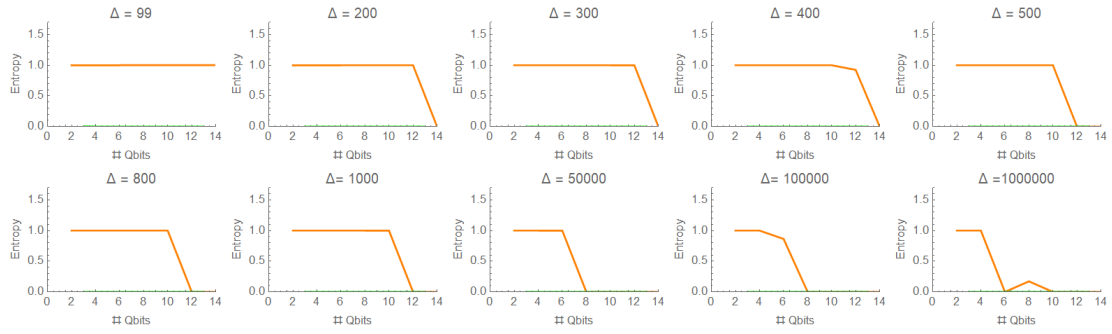

Figure 5.3: Entropy Entanglement vs. Number of Qubits for XXZ Model with $\Delta \longrightarrow \infty$

For readers who are interested in the behavior of entanglement entropy when $\Delta \longrightarrow \infty$, results are shown in Figure 5.3. As under this condition, the XXZ model approaches the

classical Ising model, and so we expect it not to be exhibiting quantum behaviour, which means that the entanglement entropy should be 0. From the graph, we could see that when Δ becomes larger, entanglement entropy vanishes at smaller number of qubits. Although the vanishing is what we expect, the phenomenon does not happen gradually, but rather happens simultaneously when some point is triggered. This seems mysterious and it left to the reader to investigate more on it.

5.1.3 Schmidt Coefficients Value Distribution

Analysis

It is natural to ask the question that how Schmidt coefficients are distributed. We would like to see that for n qubits, these 2^n coefficients follow certain trend or function. If that is the case, for a certain system, we can generate 2^n numbers from the function and treat them as Schmidt coefficients to calculate entanglement entropy. It would save much energy to calculate entanglement entropy, and would be very beneficial for investigating area law in general.

Take $\Delta = 5$ as an example since in Figure 5.2, the entanglement entropy is stable at this Δ and is not large enough for the model to approach Classical Ising model. The log plot of the Schmidt Coefficients of the ground state of the XXZ model with $\Delta = 5$ is given below. Note that the x-axis is just the order of the Schmidt Coefficients in decreasing order, i.e. the largest Schmidt Coefficient is with $x = 1$.

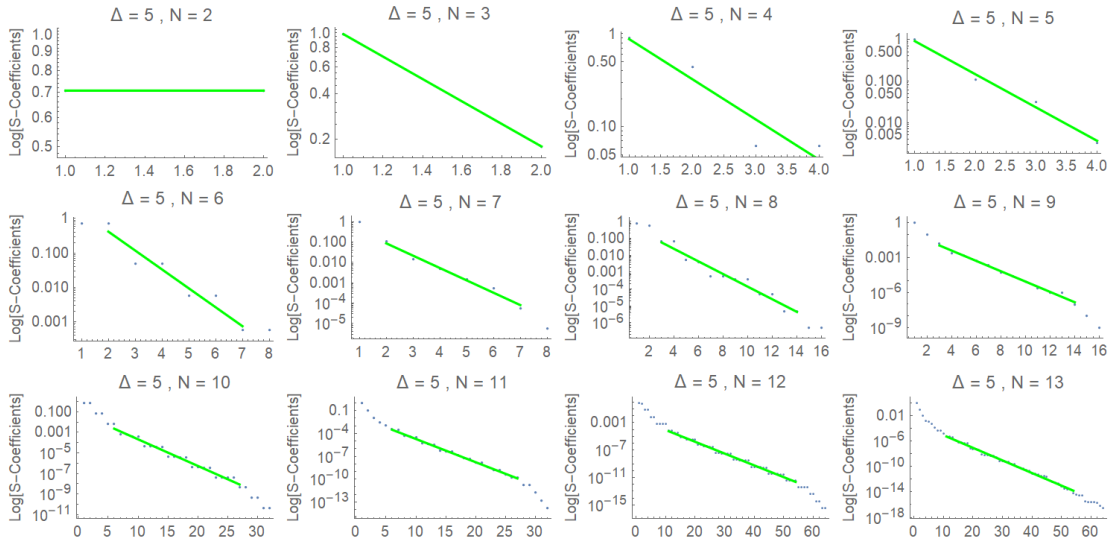

Figure 5.4: Schmidt Coefficients Value Distribution for XXZ Model with $\Delta = 5$

From the Figure 5.4, it can be deduced that Schmidt Coefficients seems to decrease exponentially (the middle of their log plots are close to be linear). We now take the assumption of

the exponential decay, and investigate how the slope of these log plots change with number of qubits n. We choose $\Delta = 3, 5, 7, 9, 11, 13, 15, 17$ as representatives.

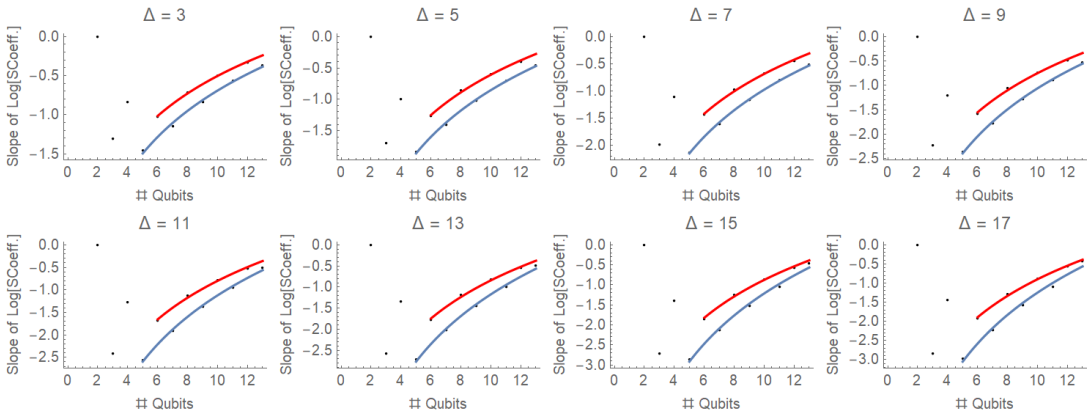

Figure 5.5: The Slope of Schmidt Coefficients Value Distribution vs. Number of Qubits for XXZ Model

Prediction

It could be seen that these functions fit the slope graph very well and we would like use these functions to predict the slope for $n = 14$. Still take $\Delta = 5$ as an example. Since from Figure 5.5, it can be seen that odd and even cases follow different log functions, as we want to predict $n = 14$, we only pay attention to the even cases for $\Delta = 5$.

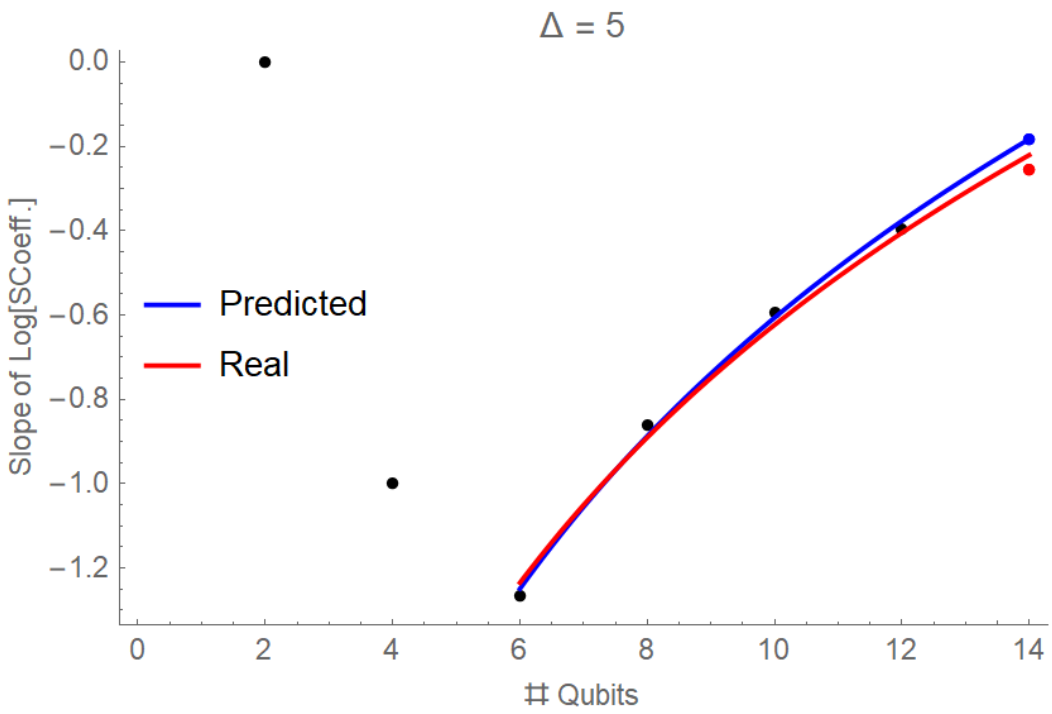

Figure 5.6: The Slope of Schmidt Coefficients Value Distribution vs. Number of Qubits for XXZ Model with $\Delta = 5$

In Figure 5.6, the blue line represents the fitting function based on $n = 6, 8, 10, 12$ and the blue point at $n = 14$ is -0.220439 and represents the predicted slope for Schmidt Coefficients value distribution for $n = 14$. The red point at $n = 14$ is -0.255295 and represents the real slope and red line represents real fitting function based on $n = 6, 8, 10, 12, 14$. The discrepancy between predicted and real slope is 0.0348554, which is not small enough.

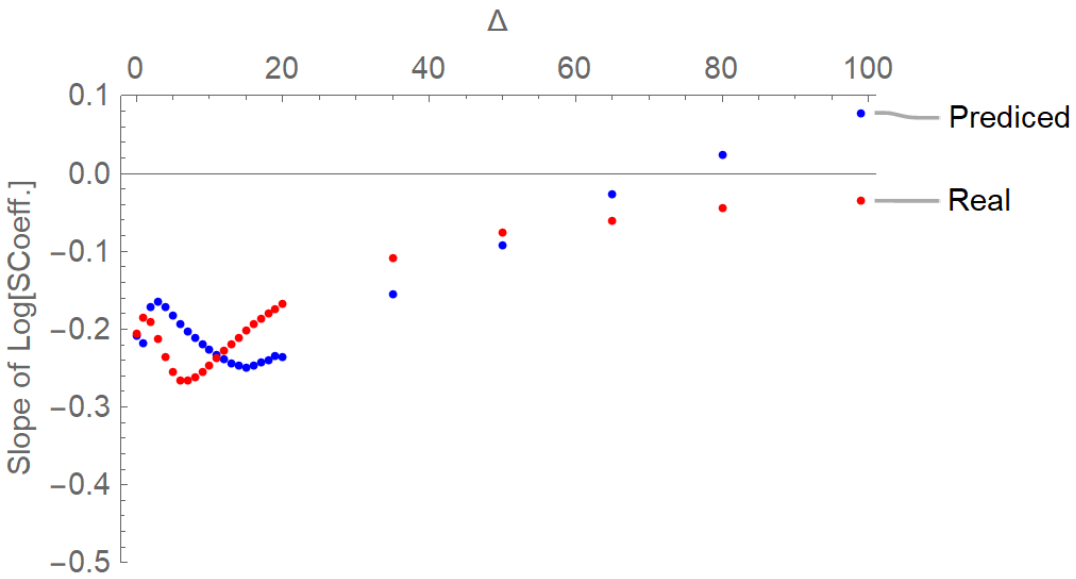

Figure 5.7: The Predicted and Real Slope of Schmidt Coefficients Value Distribution vs. Δ for XXZ Model with $n = 5$

Figure 5.7 shows the predicted and real slopes of the log of Schmidt Coefficients Value Distribution for $n = 14$ and the discrepancies are visualized for different Δ. It can be seen that for some Δ, the discrepancies are larger and even with different signs.

The imperfection of the prediction method is mainly caused by the following reason: Error: In Figure 5.4, it is clear that when n increases, the log plot of Schmidt Coefficients is more bent instead of being linear. It follows that the linear fitting function is less accurate for predicting relatively larger n. More plots like 5.4 are provided in Appendix A and it is easy to see that for some Δs the exponential decay assumption about the Schmidt Coefficients distribution is not accurate (the middle of these log plots are not linear).

Another thing to point out here is that we state in the beginning of this section that the investigation on the Schmidt Coefficients serves to better investigate the area law. As introduced in Chapter 1, the Von Neumann entropy for a bipartite ground state with the middle cut is calculated by

$$S = \sum_{i=1}^{2^{\lfloor n/2 \rfloor}} \lambda_i^2 \log \lambda_i^2,$$

where λ_i represents Schmidt Coefficients. The equation shows that larger Schmidt Coefficients contribute more to entanglement entropy and therefore it would be more beneficial to investigate larger Schmidt Coefficients' values, instead of the middle values. But in Figure 5.7, it seems that the left part of Schmidt Coefficients (larger coefficients) does not seem to follow certain simple function and might be hard to find fitting function. Readers who are interested in it are very welcome to investigate more on larger Schmidt Coefficients

distribution or even all Schmidt Coefficients distribution.

5.2 XXZ-Variant Model

5.2.1 Entropy Entanglement vs. Number of Qubits

As described in 3.2, the ground-state space of the Hamiltonian of XXZ Variant model has degeneracy $n-1$, which is not a constant, and so that it is not known for sure if an area law holds.

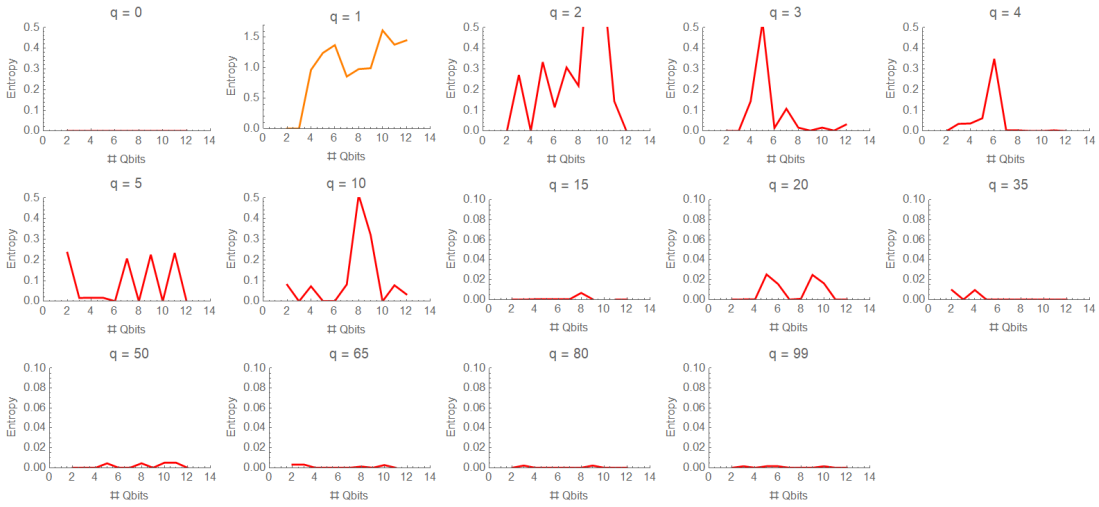

Figure 5.8: Entropy Entanglement vs. Number of Qubits for XXZ Variant Model

As proved in [15], the Hamiltonian for this model is gapped when $q \neq 1$ and so we marked $q = 1$ case in orange in Figure 5.8. It is obvious that entropy entanglement of the ground state of XXZ Variant model is not stable, although it is all below 1 for all $q \neq 1$. So we can be optimistic that this model actually follows an area law, although its instability casts some doubts on this point of view.

Since the ground state of the model is not guaranteed to follow the area law, the investigation of this model will be ended here. The information here is to provide the an example about the investigation on a frustration-free Hamiltonian.

5.3 AKLT Model

5.3.1 Entropy Entanglement vs. Number of Qubits

As described in 3.3, AKLT model is both frustration free and has constant-fold degenerate ground-state space. So it is should satisfy the area law and it is the case exactly proved in Section 2.

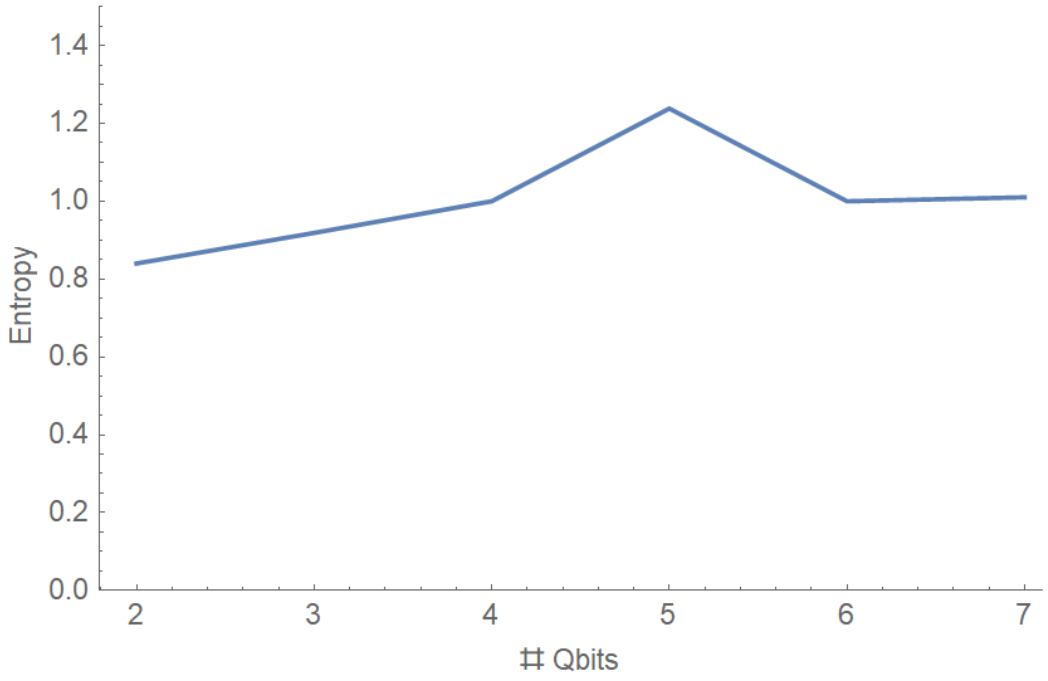

Figure 5.9: Entropy Entanglement vs. Number of Qubits for AKLT Model

In Figure 5.9, the number of qubits investigated only ranges from $n = 2$ to $n = 7$ (limited by the computational power as the dimension would be 3^n). The entropy is also not very stable with some variations and so the graph is not a good verification that AKLT follows area law.

Since the investigation is too limited by the computational power, the investigation of this model will also be ended here. The information here is to provide the an example about the investigation on a best-fit Hamiltonian (both frustation-free and has constant-fold ground state degeneracy) for proofs in Section 2.

Chapter 6

Quasi-Approximate Ground State Projector

6.1 Construction of QAGSP

As introduced in Section 2.3.2 and 2.3.5, a very common operator of interest given is $K = I - \frac{H}{\|H\|}$. K^t would give a good value of Δ with t increases, but leads to an exponential increase in Schmidt rank and hence this operator is not useful for the proof. However, we would like to study how the distribution of Schmidt coefficients related with t when K^t is applied to a random state. If there are some general trends in the Schmidt distributions with t increases, then it would be beneficial for us to get an idea of ground state entanglement entropy without calculating the ground state of the corresponding system explicitly.

By definition of AGSP, it aims to map a random state to the ground state of a certain quantum system, with bounded Schmidt rank. In this part, we would like to generalize an AGSP in terms of the identity matrix I, and the corresponding Hamiltonian H of the system ($K = I - \frac{H}{\|H\|}$ only works for frustration free Hamiltonian). We ignore the requirement of bounded Schmidt rank as it would not be satisfied using projectors like $K = I - \frac{H}{\|H\|}$. We call such project as QAGSP, standing for Quasi-Approximate Ground State Projector. Here we only want to construct AGSPs that will map ground state to ground state, and will vanish on states orthogonal to ground states, and it follows that they will map any random state to ground state(s). Definition of QAGSP is given below:

Definition 3. *An operator K is said to be a Δ-QAGSP if the following conditions hold:*

1. ***Ground space Invariance:*** *For any ground state $|\Gamma\rangle$, $K|\Gamma\rangle = |\Gamma\rangle$.*
2. ***Shrinking:*** *If $\left|\Gamma^{\perp}\right\rangle$ is any state orthogonal to the ground space, then $K\left|\Gamma^{\perp}\right\rangle$ is also orthogonal to the ground space, and moreover $||K\left|\Gamma^{\perp}\right\rangle||^2 \leq \Delta$.*

Now we show how we construct QAGSP for different models based on their eigensystems. Let the smallest eigenvalue be a and largest eigenvalue be $b > 0$ (we do not consider $b < 0$

case here), and note that $\|H\|$ is the matrix norm which means the largest absolute value of all eigenvalues here. We discuss the following cases of Hamiltonian to investigate in the following subsections.

6.1.1 Frustration Free: $a = 0$

Under this case, we can simply have $K = I - \frac{H}{\|H\|}$ as described in Section 2.3.5, such that $K|\Gamma\rangle = |\Gamma\rangle$ and $K|\Gamma^\perp\rangle = \Delta|\Gamma^\perp\rangle$ with $|\Delta| < 1$. Therefore, for a random state $|\psi\rangle$, we can have

$$\begin{aligned} K^t|\psi\rangle &= K^t\left(c_1|\Gamma\rangle + \sum_i c_i|\Gamma_i^\perp\rangle\right) \\ &= c_1^k|\Gamma\rangle + \sum_i c_i\Delta_i^k|\Gamma_i^\perp\rangle \\ &\approx c_1^k|\Gamma\rangle, \end{aligned}$$

where the last approximation comes from the fact that $\Delta^t \approx 0$ as for large enough t. After normalization, we would have $K^t|\psi\rangle \approx |\Gamma\rangle$.

6.1.2 Positive Ground State Energy: $a > 0$

Now we consider the AGSP $K = \frac{1}{1-\frac{a}{b}}\left(I - \frac{H}{\|H\|}\right)$, and we will have

$$K|\Gamma\rangle = \frac{1}{1-\frac{a}{b}}\left(I|\Gamma\rangle - \frac{H|\Gamma\rangle}{\|H\|}\right) = \frac{1}{1-\frac{a}{b}}\left(1-\frac{a}{b}\right)|\Gamma\rangle = |\Gamma\rangle.$$

For states orthogonal to the ground state, we have

$$K|\Gamma^\perp\rangle = \frac{1}{1-\frac{a}{b}}\left(I|\Gamma^\perp\rangle - \frac{H|\Gamma^\perp\rangle}{\|H\|}\right) = \frac{1-\frac{\lambda}{b}}{1-\frac{a}{b}}|\Gamma\rangle = \Delta|\Gamma^\perp\rangle,$$

where $|\Delta| < 1$ as $\lambda > a$.

Then similar to the above case, the QAGSP K^t will map a random state to the ground state.

6.1.3 Negative Ground State Energy: $a < 0$ and $|a| < b$

The case is similar to the case of $a < 0$, and so we consider the AGSP $K = \frac{1}{1-\frac{a}{b}}\left(I - \frac{H}{\|H\|}\right)$ again. It is the same for the ground state, but for states orthogonal to the ground state, we have

$$K|\Gamma^\perp\rangle = \frac{1}{1-\frac{a}{b}}\left(I|\Gamma^\perp\rangle - \frac{H|\Gamma^\perp\rangle}{\|H\|}\right) = \frac{1-\frac{\lambda}{b}}{1+\frac{|a|}{b}}|\Gamma\rangle = \Delta|\Gamma^\perp\rangle,$$

where $|\Delta| < 1$ as either $\lambda > 0$ or $|\lambda| < |a|$. Then as expected, the AGSP K^t will map a random state to the ground state.

6.1.4 Negative Ground State Energy: $a < 0$ and $|a| > b$

For the last case, we consider the AGSP $K = \frac{1}{2}\left(I - \frac{H}{\|H\|}\right)$, and we will have

$$K|\Gamma\rangle = \frac{1}{2}\left(I|\Gamma\rangle - \frac{H|\Gamma\rangle}{\|H\|}\right) = \frac{1}{2}\left(1 - \frac{a}{|a|}\right)|\Gamma\rangle = \frac{1}{2}\left(1 + \frac{|a|}{|a|}\right)|\Gamma\rangle = |\Gamma\rangle.$$

For states orthogonal to the ground state, we have

$$K\left|\Gamma^{\perp}\right\rangle = \frac{1}{2}\left(I\left|\Gamma^{\perp}\right\rangle - \frac{H\left|\Gamma^{\perp}\right\rangle}{\|H\|}\right) = \frac{1 - \frac{\lambda}{|a|}}{2}|\Gamma\rangle = \Delta\left|\Gamma^{\perp}\right\rangle,$$

where $|\Delta| < 1$ as $-|a| < \lambda < b < |a|$ and then $-1 < \frac{\lambda}{|a|} < 1$. Then as expected, the AGSP K^t will map a random state to the ground state.

6.2 Ground State Convergence

As stated above, we construct a QAGSP for the XXZ model, which is actually always $K^t = \left(\frac{1}{1-\frac{a}{b}}\left(I - \frac{H}{\|H\|}\right)\right)^t$. We first investigate how large t should be to make K^t an AGSP. Since for odd number of qubits, the ground space has dimension 2 while for even number of qubits, the ground space only has dimension 1, it is easy to set a Δ for even cases and verify that K^t has mapped a random state to the ground state.

We choose $\Delta = 10^{-7}$ as it is the numpy.isclose tolerance. t that would make K^t satisfy QAGSP definition for different number of qubits n is given below. In other words, t given in Table 6.1 is smallest integer multiple of 10 that has $K^t|\psi\rangle - |\Gamma\rangle \leq \Delta$.

n	t
2	20
4	40
6	70
8	90
10	120

Table 6.1: t vs. n such that K^t is a QAGSP

Note that even though the starting product state is random, the value t that makes it mapped to the ground state is stable and always be the number shown in Table 6.1. For

even $2 \leq n \leq 10$,

$$t \approx 12n$$

would always make K^t a good QAGSP. However, even though t would be this large to make K^t a good QAGSP, the entropy would be stable with some smaller t'. This is shown in Figure 6.1. To show that how much influence made by randomness on t', we have three rows with different randomly chosen product state. We still take $\Delta = 5$ in XXZ model (not the same Δ in QAGSP) as an example.

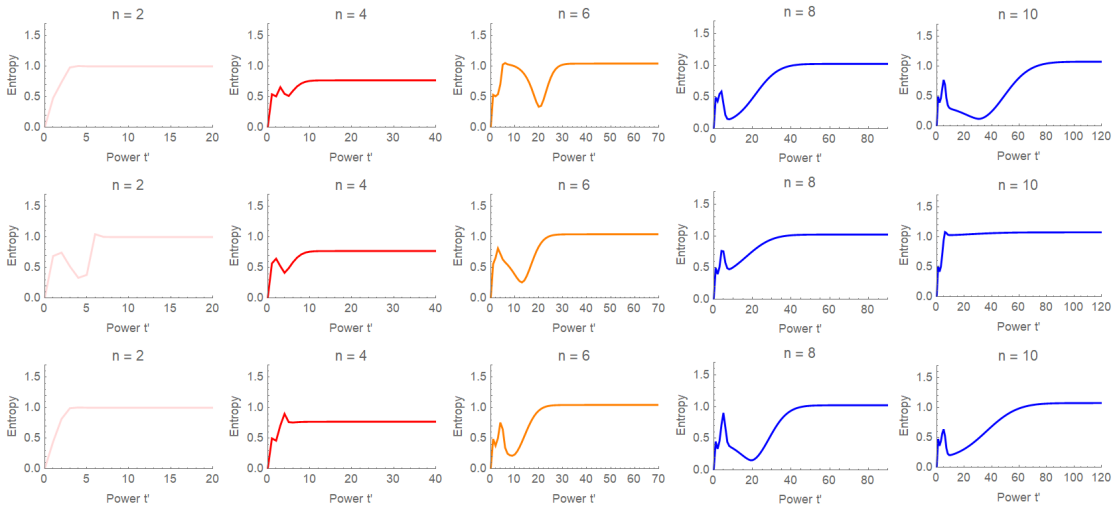

Figure 6.1: Entanglement Entropy vs. t for QAGSP of XXZ Model with $\Delta = 5$

Note that the entropy starts from 0 since a random product state has only 1 Schmidt Coefficient 1 and so has entanglement entropy 0. By comparing three rows in Figure 6.1, it could be seen that even though there are some variances in t' at which the entanglement entropy becomes stable, the entropy is always stable at

$$t' = \frac{1}{2}t \leq 6n.$$

6.3 Schmidt Coefficients Value Distribution

6.3.1 Theory on Number of Non-Zero Schmidt Coefficients

Note that a random product state has only 1 Schmidt Coefficient 1 and it can be verified in Figure 6.1 that entropy starts from 0.

The number of non-zero Schmidt Coefficients will grow until $2^{\lfloor n/2 \rfloor}$ as K is kept applying on the random states. We also claim that $|\{\lambda_i\}| \leq 5^t$ for XXZ model, where $\{\lambda_i\}$ represents the set of Schmidt Coefficients.

Proposition 6.3.1. *Let $\{\lambda_i\}$ represents the set of Schmidt Coefficients of Schmidt decomposition of $K^t |\psi_L\rangle \otimes |\psi_R\rangle$, where $|\psi_L\rangle$ and $|\psi_R\rangle$ are two random states. Then for XXZ model with n qubits,*

$$|\{\lambda_i\}| \leq \min\{5^t, 2^{\lfloor n/2 \rfloor}\}.$$

In other words, Schmidt number is smaller than or equal to 5^t.

Proof.

First, it is trivial that Schmidt number of a state should be $\leq 2^{\lfloor n/2 \rfloor}$ with the middle cut given by the procedure of Schmidt coefficients.

Second, for whatever K in Section 6.1 we finally use (even though for XXZ, we use the third one), K would always look like $c\left(I - \frac{H}{\|H\|}\right)$, where c is some scalar which has no influence on the Schmidt number. Also I and $\|H\|$ also does not influence the Schmidt number. So it suffices to consider how the Schmidt number of $H^t |\psi_L\rangle \otimes |\psi_R\rangle$ grows with t and if that is at most 5^t, we are done.

$$\begin{aligned}
H |\psi_L\rangle \otimes |\psi_R\rangle &= -\frac{J}{2} \sum_{i=1}^{n-1} \left(X_i X_{i+1} + Y_i Y_{i+1} + \Delta Z_i Z_{i+1}\right) |\psi_L\rangle \otimes |\psi_R\rangle \\
&= \left(H_L |\psi_L\rangle\right) \otimes |\psi_R\rangle \\
&\quad - \frac{J}{2} \left(X_{(n-1)/2} X_{(n+1)/2} + Y_{(n-1)/2} Y_{(n+1)/2} + \Delta Z_{(n-1)/2} Z_{(n+1)/2}\right) |\psi_L\rangle \otimes |\psi_R\rangle \\
&\quad + |\psi_L\rangle \otimes \left(H_R |\psi_R\rangle\right) \\
&= \left(H_L |\psi_L\rangle\right) \otimes |\psi_R\rangle - \frac{J}{2} X_{(n-1)/2} |\psi_L\rangle \otimes X_{(n+1)/2} |\psi_R\rangle - \frac{J}{2} Y_{(n-1)/2} |\psi_L\rangle \otimes Y_{(n+1)/2} |\psi_R\rangle \\
&\quad - \frac{J}{2} \Delta Z_{(n-1)/2} |\psi_L\rangle \otimes Z_{(n+1)/2} |\psi_R\rangle + |\psi_L\rangle \otimes \left(H_R |\psi_R\rangle\right)
\end{aligned}$$

Given by above equation, for $t = 1$, $H^t = H$ maps a product state to 5 product states. Then $H^2 |\psi_L\rangle \otimes |\psi_R\rangle = H \circ (H |\psi_L\rangle \otimes |\psi_R\rangle)$ will first map a product state to five product states and then map each of these five states to five states. Some of these 25 states might combine, and therefore H^2 will map a product states to at most 25 states. Inductively following this idea, H^t will map a product state to at most 5^t products. Formally, if we Schmidt decompose $H^t |\psi_L\rangle \otimes |\psi_R\rangle$, we will get

$$|\{\lambda_i\}| \leq 5^t,$$

which finishes the proof.

End of proof.

The effect of Proposition 6.3.1 will be noticed clearly in figures in the next section.

6.3.2 Analysis on Schmidt Coefficients Value Distribution

We now investigate the Schmidt coefficients value distribution of $K^t |\psi_L\rangle \otimes |\psi_R\rangle$ vs. t. Still take $\Delta = 5$ as an example. We focus on $n = 10$ case since it is the largest number of qubits we can investigate by the limitation of the computational power. We evaluate Schmidt coefficients for $0 \leq t \leq 60$ since the entropy becomes stable after this t.

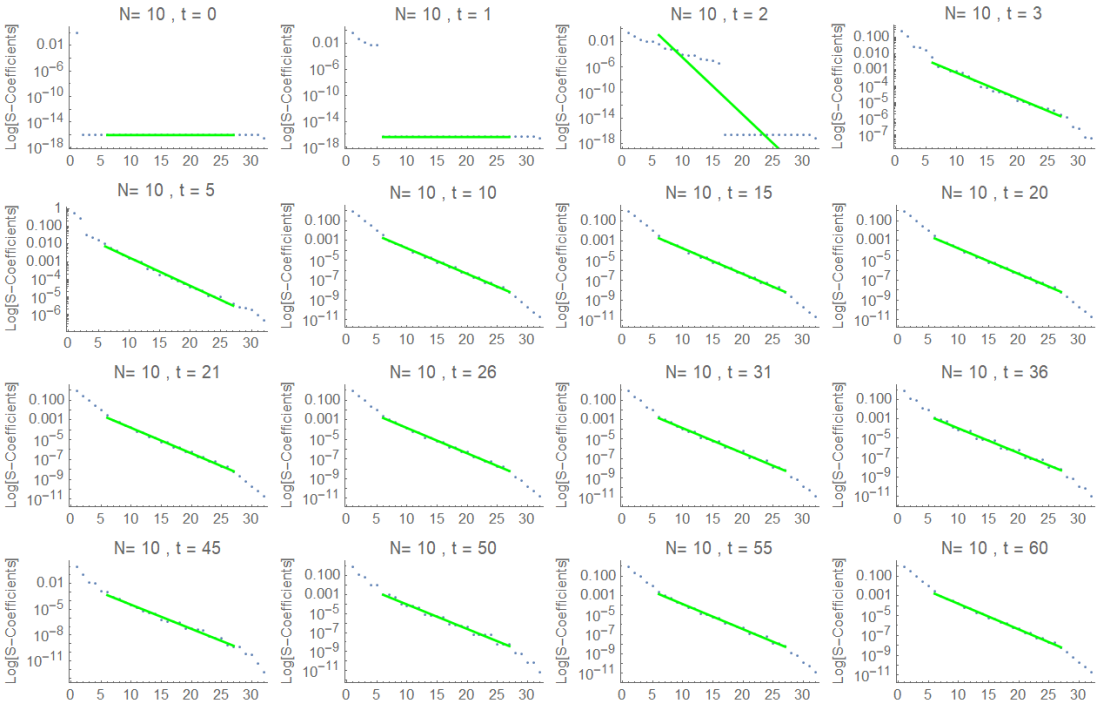

Figure 6.2: Schmidt Coefficients Value Distribution of QAGSP for XXZ Model with $\Delta = 5$

In Figure 6.2, Proposition 6.3.1 is clearly shown. For $t = 0$, there is only 1 non-zero Schmidt coefficient as expected. For $t = 1$, there are 5 non-zero Schmidt coefficients as expected. For $t = 2$, there are $16 \leq 25$ non-zero Schmidt coefficients as expected. For $t \geq 3$, $5^3 = 125 \geq 2^5 = 32$ and so all Schmidt coefficients are non zero as shown in the Figure.

Similar to Figure 6.2, it can be deduced that Schmidt coefficients seems to decrease exponentially (the middle of their log plots are close to be linear). We now take the assumption of the exponential decay again, and investigate how the slope of these log plots change with number of qubits n. All figures after correspond to log plots for Schmidt coefficients. Note that such assumption has same disadvantages as explained in the end of Section 5.1.3.

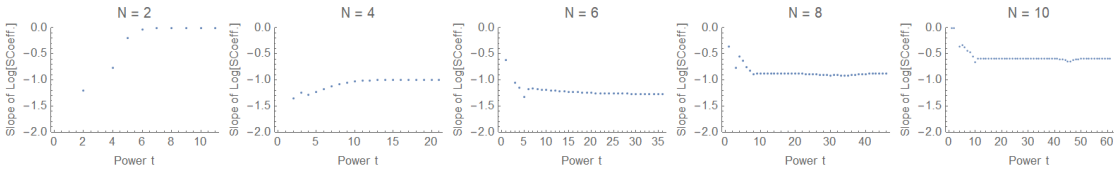

Figure 6.3: The Slope of Schmidt Coefficients Value Distribution of QAGSP vs. t for XXZ Model

The Plot with $n = 10$ in Figure 6.3 represents the slope of these value distributions in Figure 6.2. It is reasonable that after some t, the slope converges, which is because the Schmidt coefficients at that t becomes closer to the ground state and tends to be stable.

We noticed that such t is around 10. This makes us wonder whether the slope at $t = 10$ follows some rule and if that is the case, we can predict the slope at $t = 10$ for $n = 12$. Then since the slope becomes stable at $t = 10$, we can use this slope to deduce the slope of Schmidt coefficients value distribution of $K^t |\psi_L\rangle \otimes |\psi_R\rangle \approx |\Gamma\rangle$, where $|\Gamma\rangle$ represents the ground state. This prediction is the same as what we did in Section 5.1.3, i.e. to predict the slope of Schmidt coefficients value distribution for larger number of qubits n.

The experiment of the idea on the slope at $t = 10$ vs number of qubits n is given below:

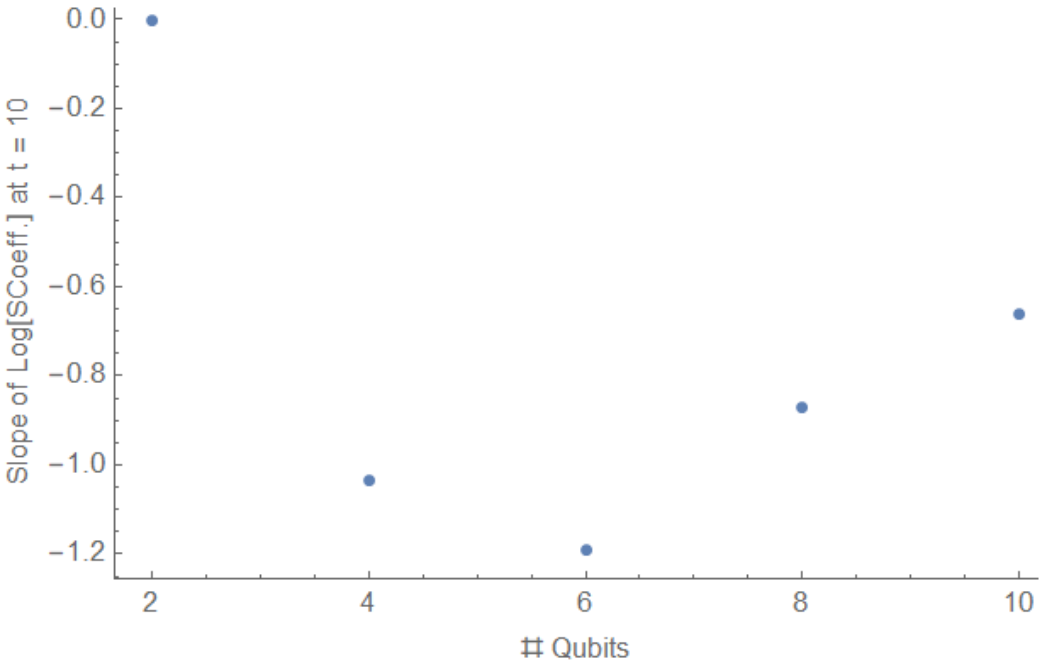

Figure 6.4: The Slope of Schmidt Coefficients Value Distribution of QAGSP vs. n for XXZ Model at $t = 10$

Unfortunately, there is no obvious relationship between these slopes at $t = 10$, which makes our hope not so achievable. This is just an idea of what we can do to predict Schmidt coefficients related information for larger n. Readers who are interested in this are welcome to implement faster algorithms like DMRG introduced in Section 4.3 to generate more qubits and that might give more ideas on the relationship, which would be beneficial for predictions.

Conclusion

The von Neumann entanglement entropy of ground states in XXZ model is verified to follow a 1D area law, i.e. the entropy is $\mathcal{O}(1)$. The entropy bound is verified to be a constant for up to 14 qubits with $1 < \Delta < \infty$, independent of the position of the cut. The Schmidt coefficients of ground states of XXZ model in decreasing order are investigated to be largely likely to follow exponential decay with up to 13 qubits. Slopes of logplot of the Schmidt coefficients value distribution are studied to predict the slope of the logplot of Schmidt coefficients distribution of 14 qubits. Discrepancies are within 0.1 for $2 \leq \Delta \leq 80$, and is mostly caused by the fact that Schmidt coefficients no longer follow exponential decay with more qubits and larger Δs.

Quasi-approximate ground state projectors $K^t = \left[c\left(I - \frac{H}{\|H\|}\right)\right]^t$, where c is some constant depending on the eigenvalues of quantum systems, is proposed to study the Schmidt coefficients and entanglement entropy. QAGSP is aimed to map random product states to ground states gradually with increased t. Schmidt coefficients distribution of $K^t |\psi\rangle$ are shown to be also largely likely to follow exponential decay for even number of qubits up to 10. Slopes of log plot of the Schmidt coefficients value distribution are also studied, but sample sizes are too small ($n = 2, 4, 6, 8, 10$) to give instructive relations between slopes and number of qubits n.

4.1 Possible Improvements

The first thing to note is that Algorithm 1 and 2 for large Δs ($\Delta \geq 10000$) give different von Neumann entropy and in Section 5.1, we use Algorithm 2 to investigate 1D area law. The Hamiltonian A_2 produced by Algorithm 2 is proved to be Hamiltonian A_1 produced by Algorithm in ground state basis, i.e. $A_2 = PA_1P^\dagger$, where P is the change of basis matrix from full basis to ground state basis. So either the numpy calcualtion of ground state of a Hamiltonian or the Schmidt decomposition will cause the discrepancies. It is worth of putting efforts to study the reason of the discrepancy of entropy calculated by these two algorithms, which is not investigated in this paper as we only care about small Δs.

The second thing is what is explained in Section 4 that both Algorithm 1 and 2 we use for investigation both generate Hamiltonians of size asymptotically $\mathcal{O}(2^n)$, which is very slow

for computation. DMRG algorithm proposed in 4.3 generates approximate Hamiltonians and other stored information that scale polynomially with respect to the size of the active space, which can be determined by investigators. Using DMRG instead of Algorithm 1 and 2 will make it possible to investigate entropy and Schmidt coefficients distribution of more qubits. It is then more possible to see the how Schmidt coefficients are distributed and how these distributions might vary with number of qubits.

Schmidt coefficients value distribution analysis in both Section 5.1.3 and Section 6.3 have two problems: lack of sample size (the investigation is only on number of qubits up to $n = 14$) and incorrect focus on the middle values of Schmidt coefficients. Detailed explanation of these two problems are in the end of Section 5.1.3 and these imperfection can be improved by implementing DMRG to increase number of qubits.

Both XXZ Variant model and AKLT model introduced in Section 3.2 and Section 3.3 are good candidates for investigating 1D area law. XXZ Variant model is good for investigating how the entanglement entropy increase with number of qubits for non constant-fold degeneracy. AKLT model is a good candidate for investigate 1D area law proof in [6] as it is both gapped and frustration free. Note that in [28], it is showed that the von Neumann entropy is saturated with the number of qubits goes to infinity theoretically. But Figure 5.9 does not show this saturation. So it might be beneficial for readers of interest to verify the 1D area law on AKLT model.

Appendix A

Schmidt Coefficients Value Distribution for Larger Δs

In Section 5.1.3, we argue that one of the imperfection of the prediction method is caused by the fact: when n increases, the log plot of Schmidt Coefficients is more bent instead of being linear. It follows that the linear fitting function of the log plot of Schmidt coefficients is not very accurate. We show log plots of Schmidt coefficients value distribution for XXZ model below, which is similar to Figure 5.4, but with larger Δs.

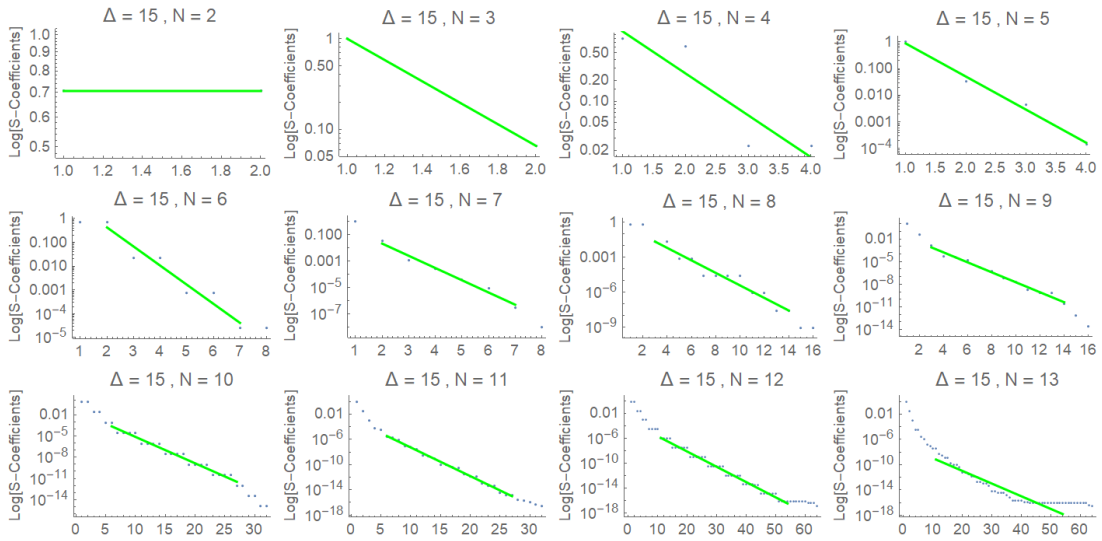

Figure A.1: Schmidt Coefficients Value Distribution for XXZ Model with $\Delta = 15$

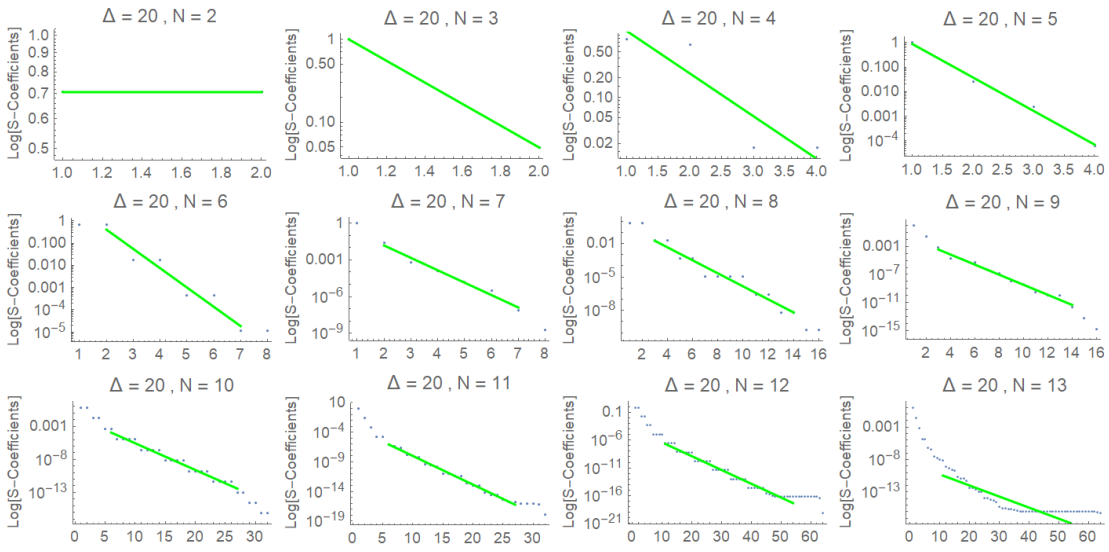

Figure A.2: Schmidt Coefficients Value Distribution for XXZ Model with $\Delta = 20$

It can be easily seen in Figure A.1 and Figure A.2 that when n increases, the log plots of Schmidt coefficients are very bent and no longer fit a straight line.

Appendix B

Code

Code used for the thesis for generating plots and investigation is provided here: `https://github.com/BiuSky7777/Reed2020-Thesis/tree/master/Code`.

Bibliography

[1] Abramowitz, M., Stegun, I. A., & Romer, R. H. (1988). Handbook of mathematical functions with formulas, graphs, and mathematical tables.

[2] Affleck, I., Kennedy, T., Lieb, E. H., & Tasaki, H. (2004). Rigorous results on valence-bond ground states in antiferromagnets. In *Condensed Matter Physics and Exactly Soluble Models*, (pp. 249–252). Springer.

[3] Aharonov, D., Arad, I., Landau, Z., & Vazirani, U. (2011). The 1d area law and the complexity of quantum states: A combinatorial approach. In *2011 IEEE 52nd Annual Symposium on Foundations of Computer Science*, (pp. 324–333). IEEE.

[4] Aharonov, D., Gottesman, D., Irani, S., & Kempe, J. (2009). The power of quantum systems on a line. *Communications in Mathematical Physics*, *287*(1), 41–65.

[5] Anshu, A., Arad, I., & Gosset, D. (2019). Entanglement subvolume law for 2d frustration-free spin systems. *arXiv preprint arXiv:1905.11337*.

[6] Arad, I., Kitaev, A., Landau, Z., & Vazirani, U. (2013). An area law and sub-exponential algorithm for 1d systems. *arXiv preprint arXiv:1301.1162*.

[7] Bethe, H. (1931). Zur theorie der metalle. *Zeitschrift für Physik*, *71*(3-4), 205–226.

[8] Bravyi, S., & Gosset, D. (2015). Gapped and gapless phases of frustration-free spin-1 2 chains. *Journal of Mathematical Physics*, *56*(6), 061902.

[9] Calabrese, P., & Cardy, J. (2004). Entanglement entropy and quantum field theory. *Journal of Statistical Mechanics: Theory and Experiment*, *2004*(06), P06002.

[10] Castro-Alvaredo, O. A., & Doyon, B. (2011). Permutation operators, entanglement entropy, and the xxz spin chain in the limit. *Journal of Statistical Mechanics: Theory and Experiment*, *2011*(02), P02001.

[11] Eckart, C., & Young, G. (1936). The approximation of one matrix by another of lower rank. *Psychometrika*, *1*(3), 211–218.

[12] Ercolessi, E., Evangelisti, S., Franchini, F., & Ravanini, F. (2011). Essential singularity in the renyi entanglement entropy of the one-dimensional xyz spin-1 2 chain. *Physical Review B*, *83*(1), 012402.

[13] Ercolessi, E., Evangelisti, S., Franchini, F., & Ravanini, F. (2012). Correlation length and unusual corrections to entanglement entropy. *Physical Review B*, *85*(11), 115428.

[14] Garcia-Saez, A., Murg, V., & Wei, T.-C. (2013). Spectral gaps of affleck-kennedy-lieb-tasaki hamiltonians using tensor network methods. *Physical Review B*, *88*(24), 245118.

[15] Gharibian, S., Huang, Y., Landau, Z., Shin, S. W., et al. (2015). Quantum hamiltonian complexity. *Foundations and Trends® in Theoretical Computer Science*, *10*(3), 159–282.

[16] Gottesman, D., & Irani, S. (2009). The quantum and classical complexity of translationally invariant tiling and hamiltonian problems. In *2009 50th Annual IEEE Symposium on Foundations of Computer Science*, (pp. 95–104). IEEE.

[17] Hastings, M. B. (2006). Solving gapped hamiltonians locally. *Physical review b*, *73*(8), 085115.

[18] Huang, Y. (2014). Area law in one dimension: Degenerate ground states and renyi entanglement entropy. *arXiv preprint arXiv:1403.0327*.

[19] Irani, S. (2010). Ground state entanglement in one-dimensional translationally invariant quantum systems. *Journal of Mathematical Physics*, *51*(2), 022101.

[20] Malvezzi, A. L. (2003). An introduction to numerical methods in low-dimensional quantum systems. *Brazilian journal of physics*, *33*(1), 55–72.

[21] Müller-Hermes, A., & Nechita, I. (2018). Operator schmidt ranks of bipartite unitary matrices. *Linear Algebra and its Applications*, *557*, 174–187.

[22] Nielsen, M. A., & Chuang, I. (2002). Quantum computation and quantum information.

[23] Parkinson, J. B., & Farnell, D. J. (2010). *An introduction to quantum spin systems*, vol. 816. Springer.

[24] Popkov, V., & Salerno, M. (2005). Logarithmic divergence of the block entanglement entropy for the ferromagnetic heisenberg model. *Physical Review A*, *71*(1), 012301.

[25] Schollwock, U. (2013). 16 dmrg: Ground states, time evolution, and spectral functions. *Emergent Phenomena in Correlated Matter*.

[26] Shannon, C. E. (1948). A mathematical theory of communication. *The Bell System Technical Journal*, *27*(3), 379–423.

[27] White, S. R. (1992). Density matrix formulation for quantum renormalization groups. *Phys. Rev. Lett.*, *69*, 2863–2866. `https://link.aps.org/doi/10.1103/PhysRevLett.69.2863`

[28] Xu, Y., Katsura, H., Hirano, T., & Korepin, V. E. (2008). Entanglement and density matrix of a block of spins in aklt model. *Journal of Statistical Physics*, *133*(2), 347–377.