The computational power of many-body systems

by

Zak Webb

A thesis
presented to the University of Waterloo
in fulfillment of the
thesis requirement for the degree of
Doctor of Philosophy
in
Physics and Astronomy (Quantum Information)

Waterloo, Ontario, Canada, 2016

© Zak Webb, 2016

Author's Declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

Abstract

This is the abstract.
Many bodied systems are weird.
They also can be used to compute things.
Yeah!

Acknowledgements

I would like to thank all the little people who made this possible.

Dedication

This is dedicated to the ones I love.

Table of Contents

List of Figures

Chapter 1

Introduction

Well known throughout physics, people talk about the 3-body problem, and its impossibility to solve. In these cases, people generally mean that there does not exist a closed form solution in general, but can we quantify exactly how hard the problem is?

In particular, if one is working with some particular many body system, how hard is it to compute various attributes about the system. I'd really like to know the answer.

While such questions have not generally been asked in physics, classifying the computation power of a problem in terms of the necessary resources in order to solve it is a foundational idea in computer science. The entire field of computational complexity arose in the attempt to classify these problems. This thesis will attempt to use tools founded in this field and apply them to the various physical systems.

1.1 Quantum walk

Over the years, randomness proved itself as a useful tool, allowing access to physical systems that are too large to accurately simulate. By assuming the dynamics of such systems can be modelled as independent events, Markov chains provide insight to the structure of the dynamics. These ideas can then be cast into the framework of random walk, where the generating Markov matrix describes the weighted, directed graph on which the walk takes place.

Using the principle of "put quantum in front," one can then analyze what happens when the random dynamics are replaced by unitary dynamics. This actually poses a little difficulty, as there is no obvious way to make a random walk have unitary dynamics. In particular, there are many ways that the particle can arrive at one particular vertex in the underlying graph, and thus after arriving at the vertex there is no way to reverse the dynamics.

There are (at least) two ways to get around this. One continues with the discrete-time structure of a random walk, and keeps track of a "direction" in addition to the position of the particle. Each step of the walk is then a movement in the chosen direction followed by a unitary update to the direction register. These Szegedy walks are extremely common in the literature, and go by the name of "discrete-time quantum walk."

Another way to get around the reversibility problem is to generalize the continuous-time model of random walks. In particular, assuming that the underlying graph is symmetric, we look at the unitary generated by taking the adjacency matrix of the graph as a Hamiltonian. This is a one-parameter family of unitaries, and thus easily reversible. The ”continuous-time quantum walk” model is the one we'll be focussing on in this thesis.

1.2 Many-body systems

Everything in nature has many particles, and the reason that physicists are so interested in smaller dynamics is the relatively understandable fact that many-body systems are extremely complicated. The entire branch of statistical physics was created in an attempt to make a coherent understanding of these large systems, since writing down the dynamics of every particle is impossible in general.

Along these lines, many models of simple interactions between particles exist in the literature. As an example, on can consider a lattice of occupation sites, where bosons can sit at any point in the lattice. Without interactions between the particles, the dynamics are easily understood as decoupled plane waves. However, by including even a simple energy penalty when multiple particles occupy the same location (i.e. particles don't like to bunch), we no longer have a closed form solution and are required to look at things such as the Bethe ansatz.

1.3 Computational complexity

While this is a physics thesis, much of my work is focused on understanding the computational power of these physical systems, and as such an understanding of the classification framework is in order. I should explain some of the motivation behind this area of research, giving a bit of background for the physicist.

These classifications are generally described by languages, or subsets of all possible 0-1 strings. In particular, given some string x, the requisite power in order to determine whether the string belongs to a language or not describes the complexity of the language.

Basically, I should define what a language is, compare with promise problems, and compare Pand NPwith BQPand QMA.

1.4 Hamiltonian Complexity

I want at least give an idea of where these results are coming from. Basically, I should mention the idea of complexity measures related to Hamiltonians, such as area laws, quantum expanders, matrix product states, etc.

Should I explain qPCP? I'm not sure. I should really just explain that this is the nice intersection between physics and CS, with a large focus on understand physical systems, and how information and computation relate to our physical world.

1.5 Layout of thesis

Most of these results have been previously published.

Chapter 2 will be taken from momentum switch/universatily paper

chapter 3 will be taken from universality paper

chapter 4 will be taken from universality paper

chapter 5 will be taken from BH-qma paper and the new one

chapter 6 will be taken from BH-qma paper and the new one

chapter 7 will have open questions from several papers.

Chapter 2

Mathematical Preliminaries

2.1 Mathematical notation

[**TO DO:** *fill this in*]

$[k] = \{1, \cdots, k\}$.

$M^{(w)} = \mathbb{I}^{\otimes w-1} \otimes M \otimes \mathbb{I}^{N-w}$

$A(G)$ is the adjacency matrix of G. $V(G)$ are the vertices of G, and $E(G)$ is the edge set of G.

$\mu(A)$ is the smallest non-zero eigenvalue of the positive semi-definite matrix A

$A\big|_{\mathcal{S}}$ is the restriction of A to the subspace $\mathcal{S}$.

2.2 Quantum information

I should at least state a couple of things.

Hadamard gate,

Circuit

universality,

etc.

2.3 Indistinguishable particles

I have a lot of things about indistinguishable particles. I should really only talk about it in one place. I think this would be a great place.

2.4 Complexity Theory

While this thesis is for the physics department, many of the results require some basic quantum complexity theory. In particular, the computer science idea for classification of computational problems in terms of the requisite resources gives a particularly nice interpretation of why certain physical systems don't equilbriate, and give a simple explanation on why certain systems do not have a known closed form solution.

This is a simple introduction, with a focus designed to make the rest of this thesis comprehensible to those without a background in complexity theory. For a more formal introduction to Complexity Theory, I would recommend [**?**], with a more in depth review found in [**?**]. For a focus on complexity as found in quantum information, I would recommend [**?**].

2.4.1 Languages and promise problems

The main foundation of computational complexity is in the classification of languages based on the requisite number of resources to determine whether some string is in a language. Unfortunately, this requires the definition of many of these terms.

In particular, what exactly is a string? Any person who has taken a basic programming class knows that a string is simply a word, but the mathematical definition is slightly more complicated. In particular, we first need to define an alphabet, and then define a string over a particular alphabet.

Definition 1 (Alphabet)**.** An alphabet is a finite collection of symbols.

Usually, an arbitrary alphabet is denoted by Γ, while the binary alphabet is denoted by $\Sigma = \{0, 1\}$. Usually, the particular alphabet has no impact on a particular complexity result, as any finite alphabet can be represented via the binary alphabet with overhead that is logarithmic in the size of the alphabet (basically, just use a binary encoding of the new alphabet).

With this definition of an alphabet, a string is simply a finite sequence of elements from the alphabet. In particular, we define Γ^n to be all length n sequences of elements from Γ, and then define

$$\Gamma^* = \bigcup_{n=0}^{\infty} \Gamma^n. \tag{2.1}$$

With this Γ^* is the set of all strings over Γ.

With this, computational complexity then deals with understanding subsets of these strings. In particular, let Π_{yes} be a subset of Γ^*. The language problem related to Π_{yes} is then to understand what resources are necessary to determine whether a given $x \in \Gamma^*$ is also contained in Π_{yes}. This can be trivial, such as for the case of $\Pi_{\text{yes}} = \Gamma^*$, or it can be impossible, such as in the case of the famous Halting Problem.

[**TO DO:** *Find halting problem stuff*]

Related to these language problems are promise problems, in which there are two subsets of Γ^*, namely Π_{yes} and Π_{no}, such that $\Pi_{\text{yes}} \cap \Pi_{\text{no}} = \emptyset$. We are then *promised* that the $x \in \Gamma^*$ that we need to sort is contained either $\Pi_{\text{yes}} \cup \Pi_{\text{no}}$. This generally opens up some more interesting problems, as without this restriction certain complexity classes do not make sense.

2.4.2 Turing machines

Up to this point, we have only discussed various classifications of strings, and stated that we will want to understand the various resources required to sort a given string into one of two different strings, but we have not explained how these resources are defined. There are various ways to do this, depending on the various computational model one is interested in, but at the highest level, we really only need to define a Turing machine.

These are a mathematical construction, that allow for the explicit definition of algorithms. In particular, they consist of a "finite-state machine" and an infinite tape. The finite-state machine is essentially just a small number of internal states, and the infinite state represents the ability to write down and then read an unbounded amount of information. The intuitive idea behind this construction is that the finite-state machine encodes some finite algorithm (which does not depend on the input to the algorithm), while the infinite tape holds the input to the problem, along with a workspace so that the Turing machine can keep track of various pieces of information.

More concretely,

[**TO DO:** *Get turing Machine stuff*]

2.4.2.1 Reductions

Note that up to this point, we have not noticed any relations between different languages.

2.4.3 Useful complexity classes

Once we have an understanding of what defines a relation, and how these are related, we can attempt to classify those languages that require different resources in order to solve.

2.4.3.1 Classical complexity classes

Perhaps the most well known question in computational complexity is the Pvs NPproblem. However, what exactly are these classes. At a most basic level, one can think of Pas those classification problems that have an efficient classical solution, while NPare those that can be checked in an efficient manner.

Definition 2 (P)**.** A promise problem ...

Definition 3 (NP)**.** A promise problem ...

2.4.3.2 Bounded-Error Quantum Polynomial Time

Intuitively, the idea behind Bounded-Error Quantum Polynomial Time (BQP) consists of those problems that can be solved by a quantum computer efficiently.

Definition 4 (BQP)**.** A promise problem $\Pi = (\Pi_{\text{yes}}, \Pi_{\text{no}})$ if there exist polynomials

2.4.3.3 Quantum Merlin-Arthur

In addition to having an understanding of when a quantum computer can solve a particular problem, we will also want an understanding of those problems that most likely cannot be

Definition 5 (QMA)**.** A promise problem $\Pi = (\Pi_{\text{yes}}, \Pi_{\text{no}})$ if there ..

2.5 Various Mathematical Lemmas

In addition to these various complexity results, it will also be useful to have a list of certain mathematical lemmas that will be used several times in the thesis. These lemmas might also be of independent interest.

2.5.1 Truncation Lemma

Perhaps the first such lemma we called the truncation lemma. The idea behind this lemma is to approximate the evolution of a state under some particular Hamiltonian with another, where the differences between the two Hamiltonians only occur far from the support of the given state. One would expect that since the state must evolve "far" in order to reach the differs between the two Hamiltonians, the evolution between the two will be close. This lemma makes this intuition precise.

Lemma 1 (Truncation Lemma)**.** *Let H be a Hamiltonian acting on a Hilbertspace $\mathcal{H}$ and let $|\,\Phi\,\rangle \in \mathcal{H}$ be a normalized state. Let $\mathcal{K}$ be a subspace of $\mathcal{H}$, let P be the projector onto $\mathcal{K}$, and let $\tilde{H} = PHP$ be the Hamiltonian within this subspace. Suppose that, for some $T > 0$, $W \in \{H, \tilde{H}\}$, $N_0 \in \natural$, and $\delta > 0$, we have, for all $0 \leq t \leq T$,*

$$e^{-iWt}|\Phi\rangle = |\gamma(t)\rangle + |\epsilon(t)\rangle \text{ with } \||\epsilon(t)\rangle\| \leq \delta$$

and

$$(1-P)H^r|\gamma(t)\rangle = 0 \text{ for all } r \in \{0, 1, \dots, N_0 - 1\}.$$

Then, for all $0 \leq t \leq T$,

$$\left\| \left(e^{-iHt} - e^{-i\tilde{H}t} \right) |\Phi\rangle \right\| \leq \left(\frac{4e\|H\|t}{N_0} + 2 \right) \left(\delta + 2^{-N_0}(1+\delta) \right).$$

This lemma actually combines two different methods. The first assumes that the

Proposition 1. *Let H be a Hamiltonian acting on a Hilbert space $\mathcal{H}$, and let $|\,\Phi\,\rangle \in \mathcal{H}$ be a normalized state. Let $\mathcal{K}$ be a subspace of $\mathcal{H}$ such that there exists an $N_0 \in \natural$ so that for all $|\,\alpha\,\rangle \in \mathcal{K}^\perp$ and for all $n \in \{0, 1, 2, \dots, N_0 - 1\}$, $\langle\,\alpha\,|H^n|\,\Phi\,\rangle = 0$. Let P be the projector onto $\mathcal{K}$ and let $\tilde{H} = PHP$ be the Hamiltonian within this subspace. Then*

$$\|e^{-it\tilde{H}}|\,\Phi\,\rangle - e^{-itH}|\,\Phi\,\rangle\| \leq 2\left(\frac{e\|H\|t}{N_0}\right)^{N_0}.$$

Proof. Define $|\,\Phi(t)\,\rangle$ and $|\,\tilde{\Phi}(t)\,\rangle$ as

$$|\,\Phi(t)\,\rangle = e^{-itH}|\,\Phi\,\rangle = \sum_{k=0}^{\infty}\frac{(-it)^k}{k!}H^k|\,\Phi\,\rangle \qquad |\,\tilde{\Phi}(t)\,\rangle = e^{-it\tilde{H}}|\,\Phi\,\rangle = \sum_{k=0}^{\infty}\frac{(-it)^k}{k!}\tilde{H}^k|\,\Phi\,\rangle.$$

Note that by assumption, $\tilde{H}^k|\,\Phi\,\rangle = H^k|\,\Phi\,\rangle$ for all $k < N_0$, and thus the first N_0 terms in the two above sums are equal. Looking at the difference between these two states, we have

$$\begin{aligned}
\||\,\Phi(t)\,\rangle - |\,\tilde{\Phi}(t)\,\rangle\| &= \left\| \sum_{k=0}^{\infty} \frac{(-it)^k}{k!} \left(H^k - \tilde{H}^k\right) |\,\Phi\,\rangle \right\| \\
&= \left\| \sum_{k=0}^{N_0-1} \frac{(-it)^k}{k!} \left(H^k - \tilde{H}^k\right) |\,\Phi\,\rangle - \sum_{k=N_0}^{\infty} \frac{(-it)^k}{k!} \left(H^k - \tilde{H}^k\right) |\,\Phi\,\rangle \right\| \\
&\le \sum_{k=N_0}^{\infty} \frac{t^k}{k!} \left(\|H\|^k + \|\tilde{H}\|^k\right) \\
&\le 2 \sum_{k=N_0}^{\infty} \frac{t^k}{k!} \|H\|^k
\end{aligned}$$

where the last step uses the fact that $\|\tilde{H}\| \le \|P\|\|H\|\|P\| = \|H\|$. Thus for any $c \ge 1$, we have

$$\begin{aligned}
\||\,\Phi(t)\,\rangle - |\,\tilde{\Phi}(t)\,\rangle\| &\le \frac{2}{c^{N_0}} \sum_{k=N_0}^{\infty} \frac{(ct)^k}{k!} \|H\|^k \\
&\le \frac{2}{c^{N_0}} \exp(ct\|H\|).
\end{aligned}$$

We obtain the best bound by choosing $c = N_0/\|Ht\|$, which gives

$$\||\,\Phi(t)\,\rangle - |\,\tilde{\Phi}(t)\,\rangle\| \le 2 \left(\frac{e\|H\|t}{N_0}\right)^{N_0}$$

as claimed. (If $c < 1$ then the bound is trivial.) □

Proposition 2. *Let $U_1, \ldots, U_n$ and $V_1, \ldots, V_n$ be unitary operators. Then for any $|\,\psi\,\rangle$,*

$$\left\| \left(\prod_{i=n}^{1} U_i - \prod_{i=n}^{1} V_i \right) |\,\psi\,\rangle \right\| \le \sum_{j=1}^{n} \left\| (U_j - V_j) \prod_{i=j-1}^{1} U_i |\,\psi\,\rangle \right\|. \tag{2.2}$$

Proof. The proof is by induction on n. The case $n = 1$ is obvious. For the induction step, we have

$$\begin{aligned}
\left\| \left(\prod_{i=n}^{1} U_i - \prod_{i=n}^{1} V_i \right) |\,\psi\,\rangle \right\| &= \left\| \left(\prod_{i=n}^{1} U_i - V_n \prod_{i=n-1}^{1} U_i + V_n \prod_{i=n-1}^{1} U_i - \prod_{i=n}^{1} V_i \right) |\,\psi\,\rangle \right\| && (2.3) \\
&\le \left\| (U_n - V_n) \prod_{i=n-1}^{1} U_i |\,\psi\,\rangle \right\| + \left\| \left(\prod_{i=n-1}^{1} U_i - \prod_{i=n-1}^{1} V_i \right) |\,\psi\,\rangle \right\| && (2.4) \\
&\le \sum_{j=1}^{n} \left\| (U_j - V_j) \prod_{i=j-1}^{1} U_i |\,\psi\,\rangle \right\| && (2.5)
\end{aligned}$$

where the last step uses the induction hypothesis. □

Proof of Lemma 1. For $M \in \natural$ write

$$\begin{aligned}
\|(e^{-iHt} - e^{-i\tilde{H}t})|\,\Phi\,\rangle\| &= \left\| \left(\left(e^{-iH\frac{t}{M}}\right)^M - \left(e^{-i\tilde{H}\frac{t}{M}}\right)^M \right) |\,\Phi\,\rangle \right\| \\
&\leq \sum_{j=1}^{M} \left\| \left(e^{-iH\frac{t}{M}} - e^{-i\tilde{H}\frac{t}{M}} \right) e^{-iW(j-1)\frac{t}{M}} |\,\Phi\,\rangle \right\| \\
&\leq \sum_{j=1}^{M} \left\| \left(e^{-iH\frac{t}{M}} - e^{-i\tilde{H}\frac{t}{M}} \right) \left(|\,\gamma(\tfrac{(j-1)t}{M})\,\rangle + |\,\epsilon(\tfrac{(j-1)t}{M})\,\rangle \right) \right\| \\
&\leq 2M\delta + \sum_{j=1}^{M} \left\| \left(e^{-iH\frac{t}{M}} - e^{-i\tilde{H}\frac{t}{M}} \right) \frac{|\,\gamma(\frac{(j-1)t}{M})\,\rangle}{\left\| |\,\gamma(\frac{(j-1)t}{M})\,\rangle \right\|} \right\| \left\| |\,\gamma(\tfrac{(j-1)t}{M})\,\rangle \right\| \\
&\leq 2M\delta + 2M \left(\frac{e\|H\|t}{MN_0} \right)^{N_0} (1+\delta)
\end{aligned}$$

where in the second line we have used Proposition **??** and in the last step we have used Proposition **??** and the fact that $\||\gamma(t)\rangle\| \leq 1 + \delta$. Now, for some $\eta > 1$, choose

$$M = \left\lceil \frac{\eta e\|H\|t}{N_0} \right\rceil$$

for $0 < t \leq T$ to get

$$\begin{aligned}
\|(e^{-iHt} - e^{-i\tilde{H}t})|\,\Phi\,\rangle\| &\leq 2M \left(\delta + \eta^{-N_0}(1+\delta) \right) \\
&\leq 2 \left(\frac{\eta e\|H\|t}{N_0} + 1 \right) \left(\delta + \eta^{-N_0}(1+\delta) \right).
\end{aligned}$$

The choice $\eta = 2$ gives the stated conclusion. □

Note that it would be slightly better to take a smaller value of η. However, this does not significantly improve the final result; the above bound is simpler and sufficient for our purposes.

2.5.2 Nullspace Projection Lemma

When we discuss the ground spaces and ground energies of various Hamiltonians, we will often want to know what happens to the ground spaces and ground energies when two such Hamiltonians are added together (such as adding penalties enforcing particular initial states). As such, the Nullspace Projection Lemma exactly discusses how such systems add together. As far as I am aware this lemma was initially used (implicitly) by Mizel et. al. [**TO DO:** *find correct reference*] We then used this in our proof of the QMA-completeness for the Bose-Hubbard model. We then found an additional place that used a similar lemma, with slightly better bounds. While the improvement is minor, here is a proof of the improved bound (and note that the improvement was left as a proof for the reader in the newer result).

Lemma 2 (Nullspace Projection Lemma)**.** *Let H_A and H_B be positive semi-definite matrices. Suppose that the nullspace, S, of H_A is nonempty, and that*

$$\gamma\big(H_B|_S\big) \geq c > 0 \qquad \textit{and} \qquad \gamma(H_A) \geq d > 0. \tag{2.6}$$

Then,

$$\gamma(H_A + H_B) \geq \frac{cd}{d + \|H_B\|}. \tag{2.7}$$

Proof. Let $|\psi\rangle$ be a normalized state satisfying

$$\langle\psi|H_A + H_B|\psi\rangle = \gamma(H_A + H_B). \tag{2.8}$$

Let Π_S be the projector onto the nullspace of H_A. First suppose that $\Pi_S|\psi\rangle = 0$, in which case

$$\langle\psi|H_A + H_B|\psi\rangle \geq \langle\psi|H_A|\psi\rangle \geq \gamma(H_A) \tag{2.9}$$

and the result follows. On the other hand, if $\Pi_S|\psi\rangle \neq 0$ then we can write

$$|\psi\rangle = \alpha|a\rangle + \beta|a^\perp\rangle \tag{2.10}$$

with $|\alpha|^2 + |\beta|^2 = 1$, $\alpha \neq 0$, and two normalized states $|a\rangle$ and $|a^\perp\rangle$ such that $|a\rangle \in S$ and $|a^\perp\rangle \in S^\perp$. (If $\beta = 0$ then we may choose $|a^\perp\rangle$ to be an arbitrary state in $S^\perp$ but in the following we fix one specific choice for concreteness.) Note that any state $|\phi\rangle$ in the nullspace of $H_A + H_B$ satisfies $H_A|\phi\rangle = 0$ and hence $\langle\phi|a^\perp\rangle = 0$. Since $\langle\phi|\psi\rangle = 0$ and $\alpha \neq 0$ we also see that $\langle\phi|a\rangle = 0$. Hence any state

$$|f(q,r)\rangle = q|a\rangle + r|a^\perp\rangle \tag{2.11}$$

is orthogonal to the nullspace of $H_A + H_B$, and

$$\gamma(H_A + H_B) = \min_{|q|^2+|r|^2=1} \langle f(q,r)|H_A + H_B|f(q,r)\rangle. \tag{2.12}$$

Within the subspace Q spanned by $|\,a\,\rangle$ and $|\,a^\perp\,\rangle$, note that

$$H_A|_Q = \begin{pmatrix} w & v^* \\ v & z \end{pmatrix} \qquad H_B|_Q = \begin{pmatrix} 0 & 0 \\ 0 & y \end{pmatrix} \tag{2.13}$$

where $w = \langle a|H_B|a\rangle$, $v = \langle a^\perp|H_B|a\rangle$, $y = \langle a^\perp|H_A|a^\perp\rangle$, and $z = \langle a^\perp|H_B|a^\perp\rangle$, and that we are interested in the smaller eigenvalue of

$$M = H_A|_Q + H_B|_Q = \begin{pmatrix} w & v^* \\ v & y+z \end{pmatrix}. \tag{2.14}$$

Letting ϵ_+ and ϵ_- be the two eigenvalues of M with $\epsilon_+ \geq \epsilon_-$, note that

$$\epsilon_+ = \|M\| \leq \|H_A|_Q\| + \|H_B|_Q\| \leq y + \|H_B|_Q\| \leq y + \|H_B\|, \tag{2.15}$$

where we have used the Cauchy interlacing theorem to note that $\|H_B|_Q\| \leq \|H_B\|$. Additionally, we have that

$$\epsilon_+\epsilon_- = \det(M) = w(y+z) - |v|^2 \geq wy \tag{2.16}$$

where we used the fact that $H_B|_Q$ is positive-semidefinite. Putting this together, we have that

$$\gamma(H_A + H_B) = \min_{|q|^2+|r|^2=1} \langle f(q,r)|H_A + H_B|f(q,r)\rangle = \epsilon_- \geq \frac{wy}{y + \|H_B\|}. \tag{2.17}$$

As the right hand side increased monotonically with both w and y, and as $w \geq \gamma(H_B|_S) \geq c$ and $y \geq \gamma(H_A) \geq d$, we have

$$\gamma(H_A + H_B) \geq \frac{cd}{d + \|H_B\|} \tag{2.18}$$

as required. □

Chapter 3

Scattering on graphs

Scattering has a long history of study in the physics literature. Ranging from the classical study of colliding objects to the analysis of high energy collisions of protons, studying the interactions of particles can be very interesting.

3.1 Motivation

Let us first take motivation from one of the most simple quantum systems: a free particle in one dimension. Without any potential or interactions, we have that the time independent Schrödinger equation reads

$$\frac{\partial^2}{\partial x^2}\psi(x) = -\frac{2m}{\hbar^2}E\psi(x) = -k^2\psi(x), \tag{3.1}$$

which requires the (unnormalizable) solutions,

$$\psi(x) = \exp(-ikx) \tag{3.2}$$

for real k. These *momentum states* correspond to particles travelling with momentum k along the real line, and form a basis for the possible states of the system.

If we now also include some finite-range potential, or a potential V that is non-zero only for $|x| < d$ for some range d, then outside this range the eigenstates remain unchanged. The only difference is that we will deal with a superposition of states for each energy instead of the pure momentum states. In particular, the scattering eigenbasis for this system will become

$$\psi(x) = \begin{cases} \exp(-ikx) + R(k)\exp(ikx) & x \leq -d \\ T(k)\exp(-ikx) & x \geq d \\ \phi(x,k) & |x| \leq d \end{cases} \tag{3.3}$$

for some functions $R(k)$, $T(k)$, and $\phi(x, k)$.

In addition to these scattering states, it is possible for bound states to exist. These states are only nonzero for $|x| < d$, as the potential allows for the particles to simply sit at a particular location. One of the canonical examples is a finite well in one dimension, in which depending on the depth of the well, any number of bound states can exist.

3.1.1 Infinite path

With this motivation in mind, let us now look at the discretized system corresponding to a graph. In particular, instead of a continuum of positions states in one dimension, we restrict the position states to integer values, with transport only between neighboring integers. Explicitly, the position basis for this Hilbert space can be labeled by $n \in \mathbb{N}$. In this basis, the discretized second derivative takes the form

$$\Delta^2 = \sum_{x=-\infty}^{\infty} (|\,x+1\,\rangle - 2|\,x\,\rangle + |\,x-1\,\rangle)\langle\,x\,| = \sum_{x=-\infty}^{\infty} \Big(|\,x+1\,\rangle\langle\,x\,| + |\,x-1\,\rangle\langle\,x\,|\Big) - 2\mathbb{I}. \tag{3.4}$$

If we then rescale the energy levels, we have that the identity term in the right hand side of (3.4) can be removed, so that Δ^2 on this discretized one-dimensional system is proportional to the adjacency matrix of an infinite path.

With this representation of the second derivative operator, we can then see that the time-independent Schrödinger equation then becomes

$$\Delta^2|\,\psi\,\rangle = \Big(\sum_{x=-\infty}^{\infty} \big(|\,x+1\,\rangle\langle\,x\,| + |\,x-1\,\rangle\langle\,x\,|\big) - 2\mathbb{I}\Big)|\,\psi\,\rangle = E'_{\psi}|\,\psi\,\rangle. \tag{3.5}$$

If we rescale the energy term, and then break the vector equation into its components, we find that

$$\langle\,x+1\,|\,\psi\,\rangle + \langle\,x-1\,|\,\psi\,\rangle = E_{\psi}\langle\,x\,|\,\psi\,\rangle \tag{3.6}$$

for all $x \in \mathbb{Z}$. If we then make the ansatz that $\langle\,x\,|\,\psi\,\rangle = e^{ikx}$ for some k, we find that

$$\langle\,x+1\,|\,\psi\,\rangle + \langle\,x-1\,|\,\psi\,\rangle = e^{ik}e^{ikx} + e^{-ik}e^{ikx} = E_{\psi}e^{ikx} = E_{\psi}\langle\,x\,|\,\psi\,\rangle \qquad \Rightarrow \tag{3.7}$$

$$E_{\psi} = e^{ik} + e^{-ik} = 2\cos(k). \tag{3.8}$$

If we then use the fact that E_{ψ} must be real, and that the amplitudes should not diverge to infinity as $x \to \pm\infty$, we find that the only possible values of k are between $[-\pi, \pi)$. Hence, in analogy with the continuous case, the eigenbasis of the Hamiltonian corresponds to momentum states, but where the possible momenta only range over $[-\pi, \pi)$. We represent this momentum state with momenta k as $|\,\tilde{k}\,\rangle$.

We can then talk about the "speed" of these states, which is given by

$$s = \left|\frac{dE_k}{dk}\right| = 2\sin(|k|). \tag{3.9}$$

Note that in the case of small k, we recover the linear relationship between speed and momentum. In this way, as the distance between the vertices grows smaller, we recover the continuum case.

One slight problem with this, however, is that these momentum states are not normalizable, and thus technically are not states in the Hilbert space. Additionally, there are an uncountable number of states, while the position basis contains only a countable number of basis states. It turns out that these basis elements are δ-function orthogonal, in that

$$\langle\,\tilde{k}\,|\,\tilde{p}\,\rangle = \sum_{x=-\infty}^{\infty} e^{-ikx}e^{ikp} = \sum_{x=-\infty}^{\infty} e^{i(p-k)x} = 2\pi\delta(p-k), \tag{3.10}$$

so that we can decompose the identity on this space as

$$\mathbb{I} = \sum_{x=-\infty}^{\infty} |\, x\,\rangle\langle\, x\,| = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk |\,\tilde{k}\,\rangle\langle\,\tilde{k}\,|. \tag{3.11}$$

3.2 Scattering off of a graph

Now that we understand the eigenstates of a discretized, one-dimensional, free particle, we should attempt to understand what happens when we include a finite potential. One method to do this is to add a potential function, with explicit potential energies at various vertices of the infinite path. However, if we wish to examine scattering only on unweighted graphs, we need to be a little more clever. As such, we will connect graphs in such a way that far from our changes the graph will look identical to that of an infinite path. In particular, we will eventually connect semi-infinite (i.e., infinite in only one direction) paths to a finite graph.

With this construction, the eigenvalue equation must still be satisfied along the semi-infinite paths, and thus the form of the eigenstates along the paths must still be of the form e^{ikx} for some k and x. However, we can no longer assume that k is real, as the fact that the attached semi-infinite paths are only infinite in one direction allow for an exponentially decaying amplitudes along the paths. Additionally, we can have nontrivial correlations between the amplitudes among the different paths.

Note that much of this discussion can be found in [**?**].

3.2.1 Infinite path and a Graph

In the most simple example, let us attached a graph $\widetilde{G}$ to an infinite path. In particular, we assume that $\widetilde{G}$ is attached to a single vertex of the infinite path, and that the graph is attached by adding an edge from each vertex in $S \subset V(\widetilde{G})$ to one specific vertex of the infinite path, which we label 0. Calling this new graph G, the adjacency matrix of G is then

$$A(G) = A(\widetilde{G}) + \sum_{v\in S\subset V(\widetilde{G})} |\,v\,\rangle\langle\, 0\,| + |\,0\,\rangle\langle\, v\,| + \sum_{x=-\infty}^{\infty} |\,x\,\rangle\langle\, x+1\,| + |\,x+1\,\rangle\langle\, x\,|. \tag{3.12}$$

If we then want to inspect the eigenvectors of this Hamiltonian, we find that the eigenvalue equation on the infinite path is identical to that of an infinite path without the graph attached. Hence, we can see that any eigenstate of the Hamiltonian must take the form $A_k e^{ikx} + B_{-k}e^{-ikx}$ for some k along the infinite paths.

With this assumption, we can see that there are three distinct cases for the form of the eigenstates. In particular, the eigenstate could have no amplitude along the infinite paths, being confined to the finite graph $\widehat{G}$. It could also be a normalizable state not confined to the finite graph $\widehat{G}$, in that the amplitude along the infinite paths decays exponentially. Finally, the eigenstate could be an unnormalizable state, in which case we will call the state a scattering state.

Let us assume that the state is a scattering state. Note that the eigenvalue of the state must be between $[-2, 2]$, and that the form of the eigenstate along the paths must be scalar multiples of e^{ikx} and e^{-ikx}. Explicitly, the state must be of the form

$$\langle x | \psi \rangle = \begin{cases} A_k e^{ikx} + B_k e^{ikx} & x \leq 0 \\ C_k e^{ikx} + D_k e^{ikx} & x \geq 0 \end{cases} \tag{3.13}$$

where we note that the amplitude can change at $x = 0$ since we have attached the graph $\widetilde{G}$. However, we do have that $A_k + B_k = C_k + D_k$, since the amplitude at 0 is single valued. Additionally, we have that the eigenvalue of this state is given by $2\cos(k)$. Note that we have not yet determined the form of the eigenstate inside the graph $\widetilde{G}$, but if we define $|\phi\rangle$ to be the restriction of $|\psi\rangle$ to the finite graph $\widetilde{G}$, then $|\phi\rangle$ must satisfy the equation

$$A(G)|\phi\rangle + (A_k + B_k) \sum_{v \in S} |v\rangle\langle v|\phi\rangle = 2\cos(k)|\phi\rangle, \tag{3.14}$$

where the additional term arises from the fact that the vertices in S are connected to the vertex 0. Finally, we have that

$$2\cos(k)\langle 0|\psi\rangle = Ae^{-ik} + B_k e^{ik} + C_k e^{ik} + D_k e^{-ik} + \sum_{v \in S} \langle v|\phi\rangle, \tag{3.15}$$

since the eigenvalue equation must be satisfied at 0.

While all of this seems rather complicated, we can focus on the case where $A_k = 1$ and $D_k = 0$ and the case where $A_k = 0$ and $D_k = 1$ individually, so that along one of the semi-infinite paths (corresponding to $x > 0$ or $x < 0$), the amplitude is given by e^{ikx} or e^{-ikx}. These two states correspond to the eigenstates of the infinite path with the amplitudes given by e^{-ikx} and e^{ikx}, with changes representing how adding the graph $\widetilde{G}$ affect the eigenstates.

With this assumption, let us first look at the case where $A_k = 1$ and $D_k = 0$. We then have that the eigenstates take the form

$$\langle x | \psi \rangle = \begin{cases} e^{-ikx} + B_k e^{ikx} & x \leq 0 \\ C_k e^{-ikx} & x \geq 0 \end{cases} \tag{3.16}$$

so that $1 + B_k = C_k$. Note that this is reminiscent of a scattering state, with reflection amplitude B_k and transmission amplitude C_k, so that we take this intuition.

3.2.2 General graphs

More generally, let $\widehat{G}$ be any finite graph, with $n+m$ vertices and an adjacency matrix given by the block matrix

$$A(\widehat{G}) = \begin{pmatrix} A & B^\dagger \\ B & D \end{pmatrix}, \tag{3.17}$$

where A is an $N \times N$ matrix, B is an $m \times N$ matrix, and D is an $m \times m$ matrix. When examining graph scattering, we will be interested in the graph G given by the graph-join of $\widehat{G}$ and N semi-infinite paths, with an additional edge between each of the first N vertices of $\widehat{G}$ and the first vertex of one semi-infinite path.

We shall label label the first N vertices of the graph $\widehat{G}$ as $(1,i)$, where $i \in [N]$, as these correspond to the first vertex in each semi-infinite path, and we will call these the *terminal vertices*. We refer to the other m vertices of $\widehat{G}$ as the *internal vertices* of $\widehat{G}$, and label them as $w \in [m]$, and we refer to the vertices on the N semi-infinite paths as (x,i), where $i \in [N]$ labels which infinite path the vertex is located on (corresponding to which vertex $(1,i)$ the path is attatched to), while $x \in \mathbb{N}$ and $x \geq 2$ labels the distance along the semi-infinite path the vertex is located. With this labeling of the vertices of G, the adjacency matrix of G is then given by

$$A(G) = A(\widehat{G}) + \sum_{j=1}^{N}\sum_{x=1}^{\infty}\big(|\,x,j\,\rangle\langle x+1,j\,| + |\,x+1,j\,\rangle\langle x,j\,|\big). \tag{3.18}$$

At this point, we want to examine the possible eigenstates of the matrix $A(G)$. It turns out that there are 3 different kinds of eigenstates, corresponding to the different qualitative properties of the eigenstate along the semi-infinite paths.

While we will mostly be interested in the third such type, it is important to understand the other kinds of eigenstates.

3.2.2.1 Confined bound states

The easiest states to analyze are the confined bound states, which are eigenstates in which the only nonzero amplitudes are on vertices inside the finite graph $\widehat{G}$. If any vertex on the semi-infinite paths has nonzero amplitude for some eigenstate of the Hamiltonian, then the form of the Hamiltonian forces all vertices on that path to have nonzero amplitude, and thus these confined bound states are exactly those states that have finite support in the basis of vertex states.

To find these confined bound states, we restrict our Hilbert space to the space spanned by the internal vertices of $\widehat{G}$. The states of interest then correspond to the eigenstates of D (the induced adjacency matrix of $A(G)$ when restricted to the internal vertices of $\widehat{G}$) with the additional restriction that the state lies in the nullspace of $B^\dagger$, so that we can extend this state to the full Hilbert space by simply assuming all other amplitudes are zero.

As we originally assumed that there are only m internal vertices of $\widehat{G}$, there are at most m such confined bound states. Additionally, note that there are no restrictions on the eigenvalues of these states, other than those that are inherited from any restrictions placed on it by D (such as the energy being bounded by the maximum degree of $\widehat{D}$).

3.2.2.2 Unconfined bound states

The next possible type of eigenstates are those that are not confined to the finite graph $\widehat{G}$ but are still normalizable. Since these states still have amplitude along the semi-infinite paths, we know that they must be of the form $Ae^(ikx)$, for some A and k. However, when k is not real (corresponding to a decaying amplitude along the paths), we have that

$$2\cos(k) = 2\cos(k_r + ik_i) = 2\cos(k_r)\cosh(k_i) - i\sin(k_r)\sinh(k_i). \tag{3.19}$$

Hence, if we assume that the state is normalizable, then $k_i \neq 0$, and as the adjacency matrix is Hermitian, we must have that the eigenvalue is real, forcing $k_r = \pi n$ for some $n \in \mathbb{N}$. Note that this then implies that $e^{ik} = z$, for some $z \in (-1,1) \setminus \{0\}$ (where 0 corresponds to the confined bound states).

[**TO DO:** *Finish this section, and determine whether this is finite or infinite.*]

3.2.2.3 Half-bound states

The half-bound states are the limit of the states as $\kappa \to 0$. In particular, they are those states where the amplitude along the infinite paths take the form $(\pm 1)^x$. These states aren't quite bound, in that they are not normalizable, but they are also not quite scattering states, as they correspond to non-moving scattering states. They won't play much of a role in this paper, but I did want to mention them.

3.2.2.4 Scattering states

We finally reach the point of scattering states, or those states we can use for computational tasks. We first assume that we are orthogonal to all bound states, and in particular that we are othogonal to all confined bound states. This allows us to uniquely construct the scattering states (without this assumption, if there existed a confined bound state at the appropriate energy, then we could simply add any multiple of the confined bound state to get a different scattering state).

Taking some intuition from the classical case, we will construct a set of states that correspond to sending a particle in towards the graph $\widehat{G}$ along one of the semi-infinite paths and understanding how it scatters off of the graph. Namely, for each $i \in [N]$ we will assume that there exists a state with amplitude along the i-th path of the form $e^{ikx} + S_{i,i}(k)e^{-ikx}$ for $k \in (-\pi, 0)$, and that the rest of the paths have amplitudes given by $S_{i,q}(k)e^{ikx}$. More concretely, we assume that the form of the states is given on the infinite paths by

$$\langle x, q \,|\, \mathrm{sc}_j(k) \rangle = \delta_{j,q} e^{-ikx} + S_{qj} e^{ikx}. \tag{3.20}$$

We then need to see whether such an eigenstate exists. In this case, note that S_{qj} corresponds to the transmitted amplitude along the q-th path if the particle was incident along the j-th path.

If we continue to make the assumption that these states exist, we can also write the amplitudes of the m interval vertices as a column vector, as $\vec{\psi}_i(k)$, in which $\vec{\psi}_{i(k)}$ is the projection of $|\mathrm{sc}_j(k)\rangle$ onto the internal vertices of $\widehat{G}$. We can then collect these vectors into an $N \times m$ matrix, namely

$$\Psi(k) := \begin{pmatrix} \vec{\psi}_1(k) & \vec{\psi}_2(k) & \cdots & \vec{\psi}_N(k) \end{pmatrix} \tag{3.21}$$

[**TO DO:** *check if this is correct $N \times m$ or $m \times N$*]

Noting that the amplitudes for $\vec{\mathrm{sc}_j(k)}$ on the terminal vertices is given by $e^{-ik}|1, j\rangle + S_j(k)e^{ik}$ (thinking of $S_j(k)$ as a vector), we can then collect all of the eigenvalue equations for the vertices in $\widehat{G}$ (both internal and termal) as

$$\begin{pmatrix} A & B^\dagger \\ B & D \end{pmatrix} \begin{pmatrix} e^{-ik}\mathbb{I} + S(k)e^{ik} \\ \Psi(k) \end{pmatrix} + \begin{pmatrix} e^{-2ik}\mathbb{I} + e^{2ik}S(k) \\ 0 \end{pmatrix} = 2\cos(k) \begin{pmatrix} e^{-ik}\mathbb{I} + S(k)e^{ik} \\ \Psi(k) \end{pmatrix}. \tag{3.22}$$

By examining the lower half of this matrix equation, we can see that

$$\Psi(z) = \frac{1}{2\cos(k)\mathbb{I} - D}\big(e^{-ik}B + e^{ik}BS(z)\big), \tag{3.23}$$

which gives the amplitudes of the internal vertices in terms of the scattering matrix.

If we then examine the upper half of the matrix equation, we find that

$$A\big(e^{-ik}\mathbb{I} + e^{ik}S(k)\big) + B^\dagger\Psi(k) + \big(e^{-2ik}\mathbb{I} + e^{2ik}S(z)\big) = 2\cos(k)\big(e^{-ik}\mathbb{I} + e^{ik}S(k)\big) \qquad \Rightarrow \tag{3.24}$$

$$-\left(\mathbb{I} - e^{ik}\left(A + B^\dagger\frac{1}{2\cos(k) - D}B\right)\right)S(k) = \mathbb{I} - e^{-ik}\left(A + B^\dagger\frac{1}{2\cos(k) - D}B\right). \tag{3.25}$$

Hence, if we define

$$Q(k) = \mathbb{I} - e^{ik}\left(A + B^\dagger\frac{1}{2\cos(k) - D}B\right), \tag{3.26}$$

we find that

$$S(k) = -Q(k)^{-1}Q(-k). \tag{3.27}$$

Putting this all together, we then have that the states $|\mathrm{sc}_j(k)\rangle$ exist for all k in which the matrix operations defining $S(k)$ are well defined. In particular, we take the inverse of $2\cos(k)\mathbb{I} - D$, and the inverse of $Q(k)$. These only possibly have problems when

3.2.2.5 Easier calculation of S-matrix

[**TO DO:** *come up with a better name of this cycle*]

While the above is useful for most values of $k \in (-pi, 0)$, unfortunately there are specific values of k (such as those for which D has eigenvalue $2\cos(k)$) in which the above analysis doesn't hold do to the singularity of some particular matrices. If we want to show that these scattering states exist for all $k \in (-\pi, 0)$, we need to somehow show that these singularities are just a problem of the analysis and are not intrinsic barriers to existence.

Along these lines, let us extend our analysis to complex z, instead of only focusing on the real line. As such, let us define the matrix

$$\gamma(z) := \begin{pmatrix} zA - \mathbb{I} & zB^\dagger \\ zB & zD - (1+z^2)\mathbb{I} \end{pmatrix}. \tag{3.28}$$

Note that

$$\begin{pmatrix} \mathbb{I} & zB^\dagger \\ 0 & zD - (1+z^2)\mathbb{I} \end{pmatrix} \begin{pmatrix} -Q(z) & 0 \\ \frac{z}{zD - (1+z^2)\mathbb{I}}B & \mathbb{I} \end{pmatrix} = \begin{pmatrix} -Q(z) + zB^\dagger\frac{1}{D-(z+z^{-1})}B & zB^\dagger \\ zB & zD - (1+z^2)\mathbb{I} \end{pmatrix} \tag{3.29}$$

$$= \gamma(z) \tag{3.30}$$

Additionally, if we note that the inverse of a block diagonal matrix can be written as

$$\begin{pmatrix} X & Y \\ Z & W \end{pmatrix}^{-1} = \begin{pmatrix} \left(X - YW^{-1}Z\right)^{-1} & -X^{-1}Y\left(W - ZX^{-1}Y\right)^{-1} \\ -W^{-1}Z\left(X - YW^{-1}Z\right)^{-1} & \left(W - ZX^{-1}Y\right)^{-1} \end{pmatrix}, \tag{3.31}$$

then we can see that

$$\gamma(z)^{-1} = \begin{pmatrix} -Q(z) & 0 \\ \frac{z}{zD-(1+z^2)\mathbb{I}}B & \mathbb{I} \end{pmatrix}^{-1} \begin{pmatrix} \mathbb{I} & zB^\dagger \\ 0 & zD - (1+z^2)\mathbb{I} \end{pmatrix}^{-1} \tag{3.32}$$

$$= \begin{pmatrix} -Q(z)^{-1} & 0 \\ \frac{z}{zD-(1+z^2)\mathbb{I}}BQ(z)^{-1} & \mathbb{I} \end{pmatrix} \begin{pmatrix} \mathbb{I} & -B^\dagger \frac{z}{zD-(1+z^2)\mathbb{I}} \\ 0 & \frac{1}{zD-(1+z^2)\mathbb{I}} \end{pmatrix}. \tag{3.33}$$

We can then use this to see that

$$\gamma(z)^{-1}\gamma(z^{-1}) = \begin{pmatrix} -Q(z)^{-1} & 0 \\ \frac{z}{zD-(1+z^2)\mathbb{I}}BQ(z)^{-1} & \mathbb{I} \end{pmatrix} \begin{pmatrix} \mathbb{I} & -B^\dagger \frac{z}{zD-(1+z^2)\mathbb{I}} \\ 0 & \frac{1}{zD-(1+z^2)\mathbb{I}} \end{pmatrix} \begin{pmatrix} \mathbb{I} & z^{-1}B^\dagger \\ 0 & z^{-1}D - (1+z^{-2})\mathbb{I} \end{pmatrix} \begin{pmatrix} -Q\left(z^{-1}\right) \\ \frac{z^{-1}}{z^{-1}D-(1+z^{-2})\mathbb{I}}B \end{pmatrix} \tag{3.34}$$

$$= \begin{pmatrix} -Q(z)^{-1} & 0 \\ \frac{z}{zD-(1+z^2)\mathbb{I}}BQ(z)^{-1} & \mathbb{I} \end{pmatrix} \begin{pmatrix} \mathbb{I} & 0 \\ 0 & z^{-2}\mathbb{I} \end{pmatrix} \begin{pmatrix} -Q\left(z^{-1}\right) & 0 \\ \frac{z^{-1}}{z^{-1}D-(1+z^{-2})\mathbb{I}}B & \mathbb{I} \end{pmatrix} \tag{3.35}$$

$$= \begin{pmatrix} -Q(z)^{-1} & 0 \\ \frac{z}{zD-(1+z^2)\mathbb{I}}BQ(z)^{-1} & z^{-2}\mathbb{I} \end{pmatrix} \begin{pmatrix} -Q\left(z^{-1}\right) & 0 \\ \frac{z^{-1}}{z^{-1}D-(1+z^{-2})\mathbb{I}}B & \mathbb{I} \end{pmatrix} \tag{3.36}$$

$$= \begin{pmatrix} Q(z)^{-1}Q(z^{-1}) & 0 \\ \frac{1}{D-(z+z^{-1})\mathbb{I}}B\left(z^{-2}\mathbb{I} - Q(z)^{-1}Q(z^{-1})\right) & z^{-2}\mathbb{I} \end{pmatrix} \tag{3.37}$$

$$= -\begin{pmatrix} S(z) & 0 \\ z^{-1}\Psi(s) & -z^{-2}\mathbb{I} \end{pmatrix} \tag{3.38}$$

As such, we can write we have a nice representation of the scattering matrix and the interior amplitudes in terms of the matrix γ. If we then note that

$$\gamma(z)^{-1} = \frac{1}{\det \gamma(z)} \operatorname{adj} \gamma(z) \tag{3.39}$$

where $\operatorname{adj} \gamma(z)$ is the adjugate matrix of $\gamma(z)$, then by (3.38) we can then see that the entries of $S(z)$ are rational functions of z.

[**TO DO:** *this still doesn't explain why we can define the S-matrix this way when things aren't invertable explanation*]

3.2.3 Scattering matrix properties

While the use of the γ matrix gives an explicit construction of the form of the eigenstates on the internal vertices, it is also useful to note that the scattering matrix at a particular momentum k can be expressed as

$$S(k) = -Q(z)^{-1}Q(z^{-1}), \tag{3.40}$$

where $z = e^{ik}$, and the matrices $Q(z)$ are given by

$$Q(z) = \mathbb{I} - z\Big(A + B^\dagger \frac{1}{\frac{1}{z} + z - D} B\Big). \tag{3.41}$$

Note that $Q(z)$ and $Q(z^{-1})$ commute for all $z \in \mathbb{C}$, as they can both be written as $\mathbb{I} + zH(z + z^{-1})$.

Using this expression for the scattering matrix, it is easy to see that $S(k)$ is a unitary matrix, as

$$S(k)^\dagger = -Q(z^{-1})^\dagger (Q(z)^{-1})^\dagger \tag{3.42}$$

and that

$$Q(z)^\dagger = \mathbb{I}^\dagger - z^\dagger\Big(A^\dagger + B^\dagger\Big(\frac{1}{\frac{1}{z} + z - D}\Big)^\dagger (B^\dagger)^\dagger\Big) = \mathbb{I} - z^\dagger\Big(A + B^\dagger \frac{1}{\frac{1}{z^\dagger} + z^\dagger - D} B\Big) = Q(z^\dagger) \tag{3.43}$$

and thus

$$S(k)^\dagger = -Q(z^{-1})^\dagger (Q(z)^{-1})^\dagger = -Q(z)Q(z^{-1})^{-1} = Q(z^{-1})^{-1}Q(z) = S(k)^{-1} \tag{3.44}$$

where we used the fact that $z = e^{ik}$ so that $z^\dagger = z^{-1}$, and the fact that $Q(z)$ and $Q(z^{-1})$ commute.

Additionally, we can make use of the fact that S is derived from an unweighted graph to show that the scattering matrices are symmetric. In particular, note that $Q(z)$ is symmetric for all z, since D is symmetric, symmetric matrices are closed under inversion, A is symmetric and B is a 0-1 matrix. As such, we have that

$$S(k)^T = -\big(Q(z)^{-1}Q(z^{-1})\big)^T = -Q(z^{-1})^T (Q(z)^{-1})^T \tag{3.45}$$

$$= -Q(z^{-1})Q(z)^{-1} = -Q(z)^{-1}Q(z^{-1}) = S(k) \tag{3.46}$$

where we used the fact that $Q(z)$ and $Q(z^{-1})$ commute.

Putting this together, we have that $S(k)$ is a symmetric, unitary matrix for all k.

3.2.4 Orthonormality of the scattering states

[**TO DO:** *go over this section more*]

We now establish the delta-function normalization of the scattering states. Let

$$\Pi_1 = \sum_{x=1}^{\infty} \sum_{q=1}^{N} |x, q\rangle\langle x, q|$$

$$\Pi_2 = \mathbb{I} - \sum_{x=2}^{\infty} \sum_{q=1}^{N} |x, q\rangle\langle x, q|$$

$$\Pi_3 = \sum_{q=1}^{N} |1, q\rangle\langle 1, q|.$$

We show that, for $k \in (-\pi, 0)$, $p \in (-\pi, 0)$, and $i, j \in \{1, \ldots, N\}$,

$$\langle \mathrm{sc}_i(p)|\mathrm{sc}_j(k)\rangle = \langle \mathrm{sc}_i(p)|\Pi_1 + \Pi_2 - \Pi_3|\mathrm{sc}_j(k)\rangle = 2\pi\delta_{ij}\delta(k-p). \tag{3.47}$$

First write

$$\begin{aligned}
\langle \mathrm{sc}_i(p)|\Pi_1|\mathrm{sc}_j(k)\rangle &= \sum_{x=1}^{\infty}\sum_{q=1}^{N}(\delta_{iq}e^{ipx} + S^*_{qi}(p)e^{-ipx})(\delta_{jq}e^{-ikx} + S_{qj}(k)e^{ikx}) \\
&= \frac{1}{2}\left(\delta_{ij} + \sum_{q=1}^{N} S^*_{qi}(p)S_{qj}(k)\right)\left(\sum_{x=1}^{\infty} e^{i(p-k)x} + \sum_{x=1}^{\infty} e^{-i(p-k)x}\right) \\
&\quad + \frac{1}{2}\left(\delta_{ij} - \sum_{q=1}^{N} S^*_{qi}(p)S_{qj}(k)\right)\left(\sum_{x=1}^{\infty} e^{i(p-k)x} - \sum_{x=1}^{\infty} e^{-i(p-k)x}\right) \\
&\quad + \frac{1}{2}(S^*_{ji}(p) + S_{ij}(k))\left(\sum_{x=1}^{\infty} e^{-i(p+k)x} + \sum_{x=1}^{\infty} e^{i(p+k)x}\right) \\
&\quad + \frac{1}{2}(S^*_{ji}(p) - S_{ij}(k))\left(\sum_{x=1}^{\infty} e^{-i(p+k)x} - \sum_{x=1}^{\infty} e^{i(p+k)x}\right).
\end{aligned}$$

We use the following identities for $p, k \in (-\pi, 0)$:

$$\begin{aligned}
\sum_{x=1}^{\infty} e^{i(p-k)x} + \sum_{x=1}^{\infty} e^{-i(p-k)x} &= 2\pi\delta(p-k) - 1 \\
\sum_{x=1}^{\infty} e^{i(p+k)x} + \sum_{x=1}^{\infty} e^{-i(p+k)x} &= -1 \\
\sum_{x=1}^{\infty} e^{i(p-k)x} - \sum_{x=1}^{\infty} e^{-i(p-k)x} &= i\cot\left(\frac{p-k}{2}\right) \\
\sum_{x=1}^{\infty} e^{i(p+k)x} - \sum_{x=1}^{\infty} e^{-i(p+k)x} &= i\cot\left(\frac{p+k}{2}\right).
\end{aligned}$$

These identities hold when both sides are integrated against a smooth function of p and k. Substituting, we get

$$\begin{aligned}
\langle \mathrm{sc}_i(p)|\Pi_1|\mathrm{sc}_j(k)\rangle = 2\pi\delta_{ij}\delta(p-k) &+ \delta_{ij}\left(\frac{i}{2}\cot\left(\frac{p-k}{2}\right) - \frac{1}{2}\right) \\
&+ \sum_{q=1}^{N} S^*_{qi}(p)S_{qj}(k)\left(-\frac{i}{2}\cot\left(\frac{p-k}{2}\right) - \frac{1}{2}\right) \\
&+ S^*_{ji}(p)\left(-\frac{1}{2} - \frac{i}{2}\cot\left(\frac{p+k}{2}\right)\right) \\
&+ S_{ij}(k)\left(-\frac{1}{2} + \frac{i}{2}\cot\left(\frac{p+k}{2}\right)\right)
\end{aligned} \tag{3.48}$$

where we used unitarity of the S-matrix to simplify the first term. Now turning to Π_2 we have

$$\langle \mathrm{sc}_i(p)|H\Pi_2|\mathrm{sc}_j(k)\rangle = 2\cos(p)\langle \mathrm{sc}_i(p)|\Pi_2|\mathrm{sc}_j(k)\rangle$$

and

$$\begin{aligned}\langle \mathrm{sc}_i(p)|H\Pi_2|\mathrm{sc}_j(k)\rangle = \langle \mathrm{sc}_i(p)|\Bigg(&2\cos(k)\Pi_2|\mathrm{sc}_j(k)\rangle + \sum_{q=1}^{N}(e^{-ik}\delta_{qj} + S_{qj}(k)e^{ik})|2,q\rangle \\ &- \sum_{q=1}^{N}(e^{-2ik}\delta_{qj} + S_{qj}(k)e^{2ik})|1,q\rangle\Bigg).\end{aligned}$$

Using these two equations we get

$$\begin{aligned}(2\cos(p) - 2\cos(k))\langle \mathrm{sc}_i(p)|\Pi_2|\mathrm{sc}_j(k)\rangle = &\,\delta_{ij}(e^{2ip-ik} - e^{-2ik+ip}) + S^*_{ji}(p)(e^{-2ip-ik} - e^{-2ik-ip}) \\ &+ S_{ij}(k)(e^{2ip+ik} - e^{2ik+ip}) \\ &+ \sum_{q=1}^{N} S^*_{qi}(p)S_{qj}(k)(e^{-2ip+ik} - e^{2ik-ip}).\end{aligned}$$

Noting that

$$\langle \mathrm{sc}_i(p)|\Pi_3|\mathrm{sc}_j(k)\rangle = \sum_{q=1}^{N}(\delta_{iq}e^{ip} + S^*_{qi}(p)e^{-ip})(\delta_{jq}e^{-ik} + S_{qj}(k)e^{ik}),$$

we have

$$\begin{aligned}\langle \mathrm{sc}_i(p)|\Pi_2 - \Pi_3|\mathrm{sc}_j(k)\rangle = &\,\delta_{ij}\left(\frac{e^{2ip-ik} - e^{-2ik+ip}}{2\cos(p) - 2\cos(k)} - e^{ip-ik}\right) \\ &+ S^*_{ji}(p)\left(\frac{e^{-2ip-ik} - e^{-2ik-ip}}{2\cos(p) - 2\cos(k)} - e^{-ip-ik}\right) \\ &+ S_{ij}(k)\left(\frac{e^{2ip+ik} - e^{2ik+ip}}{2\cos(p) - 2\cos(k)} - e^{ip+ik}\right) \\ &+ \sum_{q=1}^{N} S^*_{qi}(p)S_{qj}(k)\left(\frac{e^{-2ip+ik} - e^{2ik-ip}}{2\cos(p) - 2\cos(k)} - e^{-ip+ik}\right) \\ = &\,\delta_{ij}\left(\frac{1}{2} - \frac{i}{2}\cot\left(\frac{p-k}{2}\right)\right) + S^*_{ji}(p)\left(\frac{1}{2} + \frac{i}{2}\cot\left(\frac{p+k}{2}\right)\right) \\ &+ S_{ij}(k)\left(\frac{1}{2} - \frac{i}{2}\cot\left(\frac{p+k}{2}\right)\right) \\ &+ \sum_{q=1}^{N} S^*_{qi}(p)S_{qj}(k)\left(\frac{1}{2} + \frac{i}{2}\cot\left(\frac{p-k}{2}\right)\right).\end{aligned} \tag{3.49}$$

Adding equation (3.48) to equation (3.49) gives equation (3.47).

[**TO DO:** *These form an orthonormal basis if you also include the bound states, but this is Theorem 1 from Andrew and David's Levison's Theorem II paper. I'm not sure if I should include it.*]

3.3 Applications of graph scattering

3.3.1 NAND Trees

The motivating idea for understanding graph scattering was an explicit algorithm that computes the value of a NAND tree with N leaves in $\mathcal{O}(\sqrt{N})$ time. In particular, a NAND tree is a complete binary tree of depth $\log N$, where each leaf has a particular binary value. Each node of the tree is then assigned a binary value by evaluating the NAND of its children, and the value of the entire tree is the value of the root node. Classically, any randomized algorithm requires $\mathcal{O}(N^{0.753})$ queries to the roots in order to evaluate the value of the tree, and thus this gives an example of a quantum speedup.

The reason that we are interested in this is that the original algorithm uses graph scattering as the actual algorithm. In particular, a binary tree is attached to an infinite path at the root, and then additional vertices are attached to the leaves depending on whether the binary value is 0 or 1. It turns out that at energy 0 (i.e., momentum $-\pi/2$), such a tree has perfect transmission from one path to the other if the tree evaluates to 1, and perfect reflection if the tree evaluates to 0. Hence, if a wave packet with momentum centered around $-\pi/2$ is scattered off of such a graph, then if we determine the location of the particle after it has scattered we evaluate the tree.

In this case, the requisite size of the wavepacket turns out to be $\mathcal{O}(\sqrt{N})$, and thus this amount of time is required in order for the scattering to occur. This is closely related to the number of queries to the values of the input variables in order to compute the value of the tree, and thus this is a quantum algorithm that has a provable speedup over classical computing.

3.3.2 Momentum dependent actions

While the NAND trees gives a good example of how the process works, in that the scattering evaluates a binary function, we can use similar ideas in order to have nontrivial scattering behavior. In particular, the NAND tree algorithm utilizes the fact that some graph either completely reflects or transmits at one particular momenta in order to evaluate the function, but we can also create graphs that have different behaviors at different momenta, or that perfectly transmits to some subset of the attached paths (i.e., generalizations to multiple semi-infinite paths).

3.3.2.1 R/T gadgets

The easiest thing we could hope for are exactly similar to the NAND trees experiment, in that if there are only two attached semi-infite paths, then at some fixed momenta it either completely transmits, or it completely reflects. However, in contrast to the NAND tree, we will only work with a single graph, and use it to filter out some momenta.

Basically, the idea behind R/T gadgets is to perfectly transmit at some momenta, while perfectly reflecting at other momenta. This will then allow us to filter out certain unwanted wavepackets, and allow us to only deal with the momenta of interest. Further, these simple gadgets can be used as a simple building block in the construction of other graphs, allowing us to have more complicated graphs.

3.3.2.2 Momentum Switches

In addition to a simple graph that only reflects or transmits certain momenta, we can generalize the idea to a kind of routing behavior. In particular, we can attempt to construct a graph with three attached semi-infinite paths, in which when a wavepacket is incident on one particular path, it either perfectly transmits to the second path, or it perfectly transmits to the third path, depending on the incident momenta. In this way, we construct something like a momentum dependent railroad switch, sending different wavepackets to different locations.

In the grand scheme of things, this is extremely useful, as it allows for more general momentum dependent actions.

3.3.3 Encoded unitary

Finally, we can also encode unitary actions using these graphs, in that by necessity these scattering matrices must be unitary. In particular, let us examine what happens to a graph with four attached semi-infinite paths, when at some chosen momentum a wavepacket from either of the first two paths gets perfectly transmits to the last two paths. In this case, the S-matrix becomes a block matrix, with the two 2×2 blocks in the diagonal both zero matrices. As such, the off diagonal matrices must also be unitary, and if we think of the two input paths as an encoded qubit (with a wavepacket along one path corresponding to an encoded $|0\rangle$ state and a wavepacket along the other path correpsonding to an encoded $|1\rangle$ state) then this scattering procedure performs some encoded unitary transformation on the qubit.

3.4 Construction of graphs with particular scattering behavior

While we have shown that the scattering behavior of some given graph is easy to compute, finding a graph with a given scattering behavior is much more difficult. We don't even know whether such an operation is decidable, and thus constructing an efficient algorithm for finding a graph with a given scattering behavior seems unlikely. However, there are specific behaviors at particular momenta in which constructions are known, and some small sized graphs that have been found via exhaustive searches.

3.4.1 R/T gadgets

[**TO DO:** *Go over this section, and revise*]

Perhaps the most simple behavior will be two-terminal gadgets that either perfectly reflect at some particular momenta, or perfectly transmit. While this is still a rather complicated problem when the terminals can be any vertices of the graph, things become tractable when we want to only attach a graph to a single vertex of an infinite path. In this case, everything works out as expected.

We refer to the graph shown in Figure **??** as $\hat{G}$, and we write G for the full graph obtained by attaching two semi-infinite paths to terminals $(1,1)$ and $(1,2)$. As shown in the Figure, the graph $\hat{G}$ for a type 1 gadget is determined by a finite graph G_0 and a subset $P = \{p_1, \ldots, p_n\} \subseteq V(G_0)$ of its vertices, called the *periphery*. Each vertex in the periphery is connected to a vertex denoted a, and a is also connected to two terminals $(1,1)$ and $(1,2)$. A type 1 R/T gadget with $n = 1$ has only one edge between G_0 and a; in this special case we also call it a *type 2 R/T gadget* (see Figure **??**).

Looking at the eigenvalue equation for the scattering state $|{}_1(k)\rangle$ at vertices $(1,1)$ and $(1,2)$, we see that the amplitude at vertex a satisfies

$$\langle a|{}_1(k)\rangle = 1 + R(k) = T(k).$$

Thus perfect reflection at momentum k occurs if and only if $R(k) = -1$ and $\langle a|{}_1(k)\rangle = 0$, while perfect transmission occurs if and only if $T(k) = 1$ and $\langle a|{}_1(k)\rangle = 1$. Using this fact, we now derive conditions on the graph G_0 that determine when perfect transmission and reflection occur.

For type 1 gadgets, we give a necessary and sufficient condition for perfect reflection: G_0 should have an eigenvector for which the sum of amplitudes on the periphery is nonzero.

Lemma 3. *Let $\hat{G}$ be a type 1 R/T gadget. A momentum $k \in (-\pi, 0)$ is in the reflection set $\mathcal{R}$ if and only if G_0 has an eigenvector $|\chi_k\rangle$ with eigenvalue $2\cos(k)$ satisfying*

$$\sum_{i=1}^{n} \langle p_i|\chi_k\rangle \neq 0. \tag{3.50}$$

Proof. First suppose that $\hat{G}$ has perfect reflection at momentum k, i.e., $R(k) = -1$ and $\langle a|{}_1(k)\rangle = 0$. Since $\langle (1,1)|{}_1(k)\rangle = e^{-ik} - e^{ik} \neq 0$ and $\langle (1,2)|{}_1(k)\rangle = 0$, to satisfy the eigenvalue equation at vertex a, we have

$$\sum_{j=1}^{n} \langle p_j|{}_1(k)\rangle = e^{ik} - e^{-ik} \neq 0.$$

Further, since G_0 only connects to vertex a and the amplitude at this vertex is zero, the restriction of $|{}_1(k)\rangle$ to G_0 must be an eigenvector of G_0 with eigenvalue $2\cos(k)$. Hence the condition is necessary for perfect reflection.

Next suppose that G_0 has an eigenvector $|\chi_k\rangle$ with eigenvalue $2\cos(k)$ satisfying (3.50), with the sum equal to some nonzero constant c. Define a scattering state $|\psi_k\rangle$ on the Hilbert space of the full graph G with amplitudes

$$\langle v|\psi_k\rangle = \frac{e^{ik} - e^{-ik}}{c} \langle v|\chi_k\rangle$$

for all $v \in V(G_0)$, $\langle a|\psi_k\rangle = 0$, and

$$\langle (x,j)|\psi_k\rangle = \begin{cases} e^{-ikx} - e^{ikx} & j = 1 \\ 0 & j = 2 \end{cases}$$

for all $x \in \mathbb{Z}^+$.

We claim that $|\,\psi_k\,\rangle$ is an eigenvector of G with eigenvalue $2\cos(k)$. The state clearly satisfies the eigenvalue equation on the semi-infinite paths since it is a linear combination of states with momentum $\pm k$. At vertices of G_0, the state is proportional to an eigenvector of G_0, and since the state as no amplitude at a, the eigenvalue equation is also satisfied at these vertices. It remains to see that the eigenvalue equation is satisfied at a, but this follows immediately by a simple calculation.

Since $|\,\psi_k\,\rangle$ has the form of a scattering state with perfect reflection, we see that $R(k) = -1$ and $T(k) = 0$ as claimed. □

The following Lemma gives a sufficient condition for perfect transmission (which is also necessary for type 2 gadgets). Let g_0 denote the induced subgraph on $V(G_0) \setminus P$ where $P = \{p_i : i \in [n]\}$ is the periphery.

Lemma 4. *Let $\hat{G}$ be a type 1 R/T gadget and let $k \in (-\pi, 0)$. Suppose $|\,\xi_k\,\rangle$ is an eigenvector of g_0 with eigenvalue $2\cos k$ and with the additional property that, for all $i \in [n]$,*

$$\sum_{\substack{v \in V(g_0):\\ (v,p_i) \in E(G_0)}} \langle\, v\,|\,\xi_k\,\rangle = c \neq 0 \tag{3.51}$$

for some constant c that does not depend on i. Then k is in the transmission set $\mathcal{T}$. If $\hat{G}$ is a type 2 R/T gadget, then this condition is also necessary.

Proof. If g_0 has a suitable eigenvector $|\,\xi_k\,\rangle$ satisfying (3.51), define a scattering state $|\,\psi_k\,\rangle$ on the full graph G, with amplitudes $\langle a|\,\psi_k\,\rangle = 1$,

$$\langle\, v\,|\,\psi_k\,\rangle = \begin{cases} -\frac{1}{c}\langle\, v\,|\,\xi_k\,\rangle & v \in V(g_0) \\ 0 & v \in P \end{cases} \tag{3.52}$$

in the graph G_0, and

$$\langle (x,j)|\,\psi_k\,\rangle = \begin{cases} e^{-ikx} & j = 1 \\ e^{ikx} & j = 2 \end{cases}$$

for $x \in \mathbb{Z}^+$. As in the proof of Lemma 3, the state $|\,\psi_k\,\rangle$ is clearly satisfies the eigenvalue equation (with eigenvalue $2\cos(k)$) at vertices on the semi-infinite paths and vertices of g_0. The factor of $-\frac{1}{c}$ in (3.52) is chosen so that the eigenvalue condition is satisfied at vertices in P. It is easy to see that the eigenvalue condition is also satisfied at a.

Since $|\,\psi_k\,\rangle$ is a scattering eigenvector of G with eigenvalue $2\cos(k)$ and perfect transmission, we have $T(k) = 1$.

Now suppose $\hat{G}$ is a type 2 R/T gadget (as shown in Figure **??**), with $P = \{p\}$. Perfect transmission along with the eigenvalue equation at vertex a implies

$$\langle\, p\,|\,_1(k)\,\rangle = 0,$$

so the restriction of $|\,_1(k)\,\rangle$ to g_0 must be an eigenvector (since p is the only vertex connected to g_0). The eigenvalue equation at p gives

$$\langle\, a\,|\,_1(k)\,\rangle + \sum_{w:\,(w,p)\in E(G_0)} \langle\, w\,|\,_1(k)\,\rangle = 0 \quad \Longrightarrow \quad \sum_{w:\,(w,p)\in E(G_0)} \langle\, w\,|\,_1(k)\,\rangle = -1.$$

Hence the restriction of $|_1(k)\rangle$ to $V(g_0)$ is an eigenvector of the induced subgraph, with the additional property that the sum of the amplitudes at vertices connected to p is nonzero. $\square$

3.4.1.1 Explicit constructions

While the above gives a nice abstract explanation for the construction of R/T gadgets, it doesn't provide us with a concrete example without the graphs that satisfy the assumptions of the lemmas. As such, let us look at two simple graphs.

As a first example, suppose G_0 is a finite path of length $l_1 + l_2 - 2$ connected to a at the l_1th vertex, as shown in Figure **??**. We determine the reflection and transmission sets as a function of l_1 and l_2.

Using Lemma 3, we see that perfect reflection occurs at momentum $k \in (-\pi, 0)$ if and only if the path has an eigenvector with eigenvalue $2\cos(k)$ with non-zero amplitude on vertex l_1. Recall that the path of length L (where the length of a path is its number of edges) has eigenvectors $|\psi_j\rangle$ for $j \in [L+1]$ given by

$$\langle x|\psi_j\rangle = \sin\left(\frac{\pi j x}{L+2}\right) \tag{3.53}$$

with eigenvalues $\lambda_j = 2\cos(\pi j/(L+2))$. Hence

$$\mathcal{R}_{\text{path}} = \left\{-\frac{\pi j}{l_1 + l_2} : j \in [l_1 + l_2 - 1] \text{ and } \frac{j l_1}{l_1 + l_2} \notin \mathbb{Z}\right\}.$$

To characterize the momenta at which perfect transmission occurs, consider the induced subgraph obtained by removing the l_1th vertex from the path of length $l_1 + l_2 - 2$ (a path of length $l_1 - 2$ and a path of length $l_2 - 2$). We can choose bases for the eigenspaces of this induced subgraph so that each eigenvector has all of its support on one of the two paths, and has nonzero amplitude on one of the vertices $l_1 - 1$ or $l_1 + 1$. Thus Lemma 4 implies that $\hat{G}$ perfectly transmits for all momenta in the set

$$\mathcal{T}_{\text{path}} = \left\{-\frac{\pi j}{l_1} : j \in [l_1 - 1]\right\} \cup \left\{-\frac{\pi j}{l_2} : j \in [l_2 - 1]\right\}.$$

For example, setting $l_1 = l_2 = 2$, we get $\mathcal{T}_{\text{path}} = \{-\frac{\pi}{2}\}$ and $\mathcal{R}_{\text{path}} = \{-\frac{\pi}{4}, -\frac{3\pi}{4}\}$.

Now let us suppose G_0 is a cycle of length r. Labeling the vertices by $x \in [r]$, where $x = r$ is the vertex attached to the path (as shown in Figure **??**), the eigenvectors of the r-cycle are

$$\langle x|\phi_m\rangle = e^{2\pi i x m/r}$$

with eigenvalue $2\cos(2\pi m/r)$, where $m \in [r]$. For each momentum $k = -2\pi m/r \in (-\pi, 0)$, there is an eigenvector with nonzero amplitude on the vertex r (i.e., $\langle r|\phi_m\rangle \neq 0$), so Lemma 3 implies that perfect reflection occurs at each momentum in the set

$$\mathcal{R}_{\text{cycle}} = \left\{-\frac{\pi j}{r} : j \text{ is even and } j \in [r-1]\right\}.$$

To see which momenta perfectly transmit, we use Lemma 4. Consider the induced subgraph obtained by removing vertex r. This subgraph is a path of length $r - 2$ and has eigenvalues $2\cos(\pi m/r)$ for $m \in [r-1]$ as discussed in the previous section. Using the expression (3.53) for the eigenvectors, we see that the sum of the amplitudes on the two ends is nonzero for odd values of m. Perfect transmission occurs for each of the corresponding momenta:

$$\mathcal{T}_{\text{cycle}} = \left\{ -\frac{\pi j}{r} : j \text{ is odd and } j \in [r-1] \right\}.$$

For example, the 4-cycle (i.e., square) has $\mathcal{T}_{\text{cycle}} = \{-\frac{\pi}{4}, -\frac{3\pi}{4}\}$ and $\mathcal{R}_{\text{cycle}} = \{-\frac{\pi}{2}\}$.

3.4.2 Momentum switches

[**TO DO:** *Go over this section, and revise/make it fit*]

To construct momentum switches between pairs of momentum, it will be worthwhile to first construct two R/T gadgets between the two momenta, with the two gadgets having swapped reflection and transmission sets. We will then construct something like a railroad switch, by placing the two gadgets immediately after a 3-claw; this construction will then be that the wavepacket will only see one of the two outgoing paths, and function exactly how we want it to.

We now construct a momentum switch between the reflection and transmission sets $\mathcal{R}$ and $\mathcal{T}$ of a type 2 R/T gadget. We attach the gadget and its reversal (defined in Section **??**) to the leaves of a claw, as shown in Figure **??**. Specifically, given a type 2 R/T gadget $\hat{G}$, the corresponding momentum switch $\hat{G}^{\prec}$ consists of a copy of G_0, a copy of $G_0^{\leftrightarrow}$, and a claw. The three leaves of the claw are the terminals. Vertex p of G_0 is connected to leaf 2 of the claw, and vertices $w_1^{(1)}, \ldots, w_r^{(1)}$ of $G_0^{\leftrightarrow}$ are each connected to leaf 3 of the claw.

The high-level idea of the switch construction is as follows. For momenta in the transmission set, the gadget perfectly transmits while its reversal perfectly reflects, so the claw is effectively a path connecting terminals 1 and 2. For momenta in the reflection set, the roles of transmission and reflection are reversed, so the claw is effectively a path connecting terminals 1 and 3.

Lemma 5. *Let $\hat{G}$ be a type 2 R/T gadget with reflection set $\mathcal{R}$ and transmission set $\mathcal{T}$. The gadget $\hat{G}^{\prec}$ described above is a momentum switch between $\mathcal{R}$ and $\mathcal{T}$.*

Proof. We construct a scattering eigenstate for each momentum $k \in \mathcal{T}$ with perfect transmission from path 1 to path 2, and similarly construct a scattering eigenstate for each momentum $k' \in \mathcal{R}$ with perfect transmission from 1 to 3. These eigenstates show that $S_{2,1}(k) = 1$ and $S_{3,1}(k') = 1$. Since the S-matrix is symmetric and unitary, this gives the complete form of the S-matrix for all momenta in $\mathcal{R} \cup \mathcal{T}$. In particular, this shows that $\hat{G}^{\prec}$ is a momentum switch between $\mathcal{R}$ and $\mathcal{T}$.

We first construct the scattering states for momenta $k \in \mathcal{T}$. Lemma 4 shows that the graph g_0 has a $2\cos(k)$-eigenvector $|\xi_k\rangle$ satisfying equation (3.51) with some nonzero constant c. We define a state $|\mu_k\rangle$ on $G^{\prec}$ and we show that it is a scattering eigenstate with perfect transmission between paths 1 and 2. The amplitudes of $|\mu_k\rangle$ on the semi-infinite paths and the claw are

$$\langle (x,1)|\mu_k\rangle = e^{-ikx} \qquad \langle 0|\mu_k\rangle = 1 \qquad \langle (x,2)|\mu_k\rangle = e^{ikx} \qquad \langle (x,3)|\mu_k\rangle = 0.$$

The rest of the graph consists of the three copies of the subgraph g_0 and the vertices p and $u_{\leftrightarrow}$. The corresponding amplitudes are

$$\langle v | \mu_k \rangle = \begin{cases} -\frac{1}{c}\langle v | \xi_k \rangle & v \in V(g_0^{(1)}) \\ \frac{1}{c}\langle v | \xi_k \rangle & v \in V(g_0^{(2)}) \\ -\frac{e^{ik}}{c}\langle v | \xi_k \rangle & v \in V(g_0^{(3)}) \\ 0 & v = p \text{ or } v = u_{\leftrightarrow}. \end{cases}$$

We claim that $|\mu_k\rangle$ is an eigenstate of the Hamiltonian with eigenvalue $2\cos(k)$. As in previous proofs, the state clearly satisfies the eigenvalue condition on the semi-infinite paths and at the vertices of G_0 and $G_0^{\leftrightarrow}$, and the factors of $\frac{1}{c}$ in the above equation are chosen so that it also satisfies the eigenvalue condition at vertices p and $u_{\leftrightarrow}$. Since $|\mu_k\rangle$ is a scattering state with perfect transmission from path 1 to path 2, we see that $S_{2,1}(k) = 1$.

Finally, we construct an eigenstate $|\nu_{k'}\rangle$ with perfect transmission from path 1 to path 3 for each momentum $k' \in \mathcal{R}$. This state has the form

$$\langle (x,1)|\nu_{k'}\rangle = e^{-ik'x} \qquad \langle 0|\nu_{k'}\rangle = 1 \qquad \langle (x,2)|\nu_{k'}\rangle = 0 \qquad \langle (x,3)|\nu_{k'}\rangle = e^{ik'x}$$

on the semi-infinite paths and the claw. Lemma 3 shows that G_0 has a $2\cos(k')$-eigenstate $|\chi_{k'}\rangle$ with $\langle p|\chi_{k'}\rangle \neq 0$, which determines the form of $|\nu_{k'}\rangle$ on the remaining vertices:

$$\langle v | \nu_{k'} \rangle = \begin{cases} -\frac{1}{\langle p | \chi_{k'}\rangle}\langle v | \chi_{k'} \rangle & v \in V(G_0) \\ -\frac{e^{ik'}}{\langle p | \chi_{k'}\rangle}\langle v | \chi_{k'} \rangle & v \in V(g_0^{(2)}) \\ -e^{ik'} & v = u^{\leftrightarrow} \\ 0 & \text{otherwise.} \end{cases}$$

As before, it is easy to check that this a momentum-k' scattering state with perfect transmission from path 1 to path 3, so $S_{3,1}(k') = 1$.

Thus the gadget from Figure **??** is a momentum switch between $\mathcal{R}$ and $\mathcal{T}$. $\square$

3.4.2.1 Explicit examples

[**TO DO:** *work this section*]

3.4.3 Encoded unitaries

While there is no efficient method to find graphs that apply some fixed encoded unitary, it is possible to search over all small graphs that have some particular implementation.

[**CITE:** *Find this small graphs thing*]

Essentially, the main idea behind this method is that since we can easily compute the scattering matrix for a particular graph at a particular momentum, if we want to find a graph that has some prescribed scattering behavior at a prescribed momenta we simply assume that such a graph exists with a particular number of internal vertices, and then search over all graphs of that size. While this exhaustive search is not guaranteed to find such a graph, a surprising number of systems can be found with this structure.

In particular, if we restrict ourselves to simple momenta, in which the energy $2\cos(k)$ is in some simple extension of the rationals, then most simple scattering behaviors can be found.

Graphs that end up being of particular use are those that allow for encoded unitary transformations. As such, we want to find graphs in which the attached paths can be partitioned into two sets, corresponding to input paths and output paths. We then want the scattering matrices at some particular momenta to be block matrices, with the diagonal blocks being zero matrices.

While this puts a large restriction on the graphs, many such graphs have been found. In particular [**CITE:** *small graphs scattering stuff*] has run an exhaustive search for such matrices up to size [**TO DO:** *find size*] . Some graphs that will be of particular interest to us are those that serve as a universal set of gates at two particular momenta. In particular, we will find uses for graphs that at momenta $-\frac{\pi}{4}$ implement a phase gate and implement a basis changing gate, and graphs that at momenta $-\frac{\pi}{2}$ implement a Hadamard gate.

These graphs are as follows: [**TO DO:** *show these graphs*]

3.5 Various facts about scattering

While we have the previous constructions that yield graphs with particular behavior, we will also want to understand some simple relations between graphs and their respective scattering matrices. In particular, understanding what properties are necessary in order to have a given scattering matrix, and understanding the relation between various the scattering matrices of various momenta.

3.5.1 Degree-3 graphs are sufficient

One of the most simple assumptions that could be made is that certain scattering behaviors require high degree graphs. In particular, the idea that having many connections might allow for some additional correlations between the outputs on larger graphs.

If we restrict our attention to only a finite number of rational momenta, however, this does not turn out to be the case. We can show that any graph can be replaced by a degree three graph with an identical scattering behavior at some fixed momenta. In particular, we show that a single vertex can be replaced by a finite path while still satisfying the eigenvalue equation at some fixed momenta, which determine the length of the path.

As a degree two graphs are the graph joins of cycles and paths, degree three graphs are the smallest graphs to have nontrivial scattering behaviors. This lemma shows that, in a certain sense, they are also all that are required.

Lemma 6. *Let $\widehat{G}$ be a finite graph, and let M be a finite set of rational multiples of π. If $v \in V(G)$ is a degree d vertex, there exists a graph H that extends G with the vertex v being replaced by a degree-$(\lceil \frac{d}{2} \rceil + 1)$ subgraph such that the scattering matrices at the momenta $k \in M$ are preserved.*

Proof. The main idea behind this proof is to partition the vertices adjacent to v into two sets, and then replace v by a finite path, with the two sets connected to opposites ends of the finite path. By choosing the length of the path correctly, we can show that the amplitudes at either end of the path can be taken as the same amplitude of v at each momenta in M, so that the eigenvalue equation remains satisfied with the same amplitudes on every vertex other than v, keeping the scattering matrices the same.

In particular, let v be the degree d vertex in G, and let $S = \{w \in V(G) : w \sim v\}$. Additionally, let us arbitrarily partition S into two sets, S_1 and S_2, such that $\big||S_1|-|S_2|\big| \leq 1$.

As each $k \in M$ is a finite set of rational multiples of π, there exists some $m' \in \mathbb{N}$ such that for each $k \in M$, $mk = 2\pi j$ for some $j \in \mathbb{N}$. Let us then examine the graph H where v is replaced by a path of length $m+1$ and S_1 is attached to one end of the path while S_2 is attached to the other end. Explicitly:

$$V(H) = V(G) \setminus \{v\} \cup \{(v,j) : j \in [m+1]\} \tag{3.54}$$

$$\begin{aligned} E(H) = \big\{e \in E(G) : v \notin e\big\} \cup \big\{\{(v,j),(v,j+1)\} : j \in [m]\big\} \cup \\ \big\{\{s,(v,0)\} : s \in S_1\big\} \cup \big\{\{s,(v,m)\} : s \in S_2\big\}. \end{aligned} \tag{3.55}$$

Now, for any $k \in M$, let $|\phi\rangle$ be an eigenstate of $A(G)$ with eigenvalue $2\cos(k)$. We will show that there exists an eigenstate $|\psi\rangle$ of $A(H)$ with energy $2\cos(k)$ such that for any $w \in V(G) \setminus \{v\}$, $\langle w|\phi\rangle = \langle w|\psi\rangle$. Concretely, for any vertex other than v, let us define $|\psi\rangle$ in this manner, and note that $|\psi\rangle$ satisfies the eigenvalue equation with energy $2\cos(k)$ for all vertices other than those in S or those replacing v by assumption. Additionally, let

$$\alpha = \sum_{w \in S_1} \langle w|\phi\rangle \qquad \beta = \langle v|\phi\rangle \qquad \gamma = \sum_{w \in S_2} \langle w|\phi\rangle. \tag{3.56}$$

We will then defined the amplitude along the path replacing the vertex v as

$$\langle (v,j)|\psi\rangle = \beta\cos(kj) + \frac{\gamma - \beta\cos(k)}{\sin(k)}\sin(kj). \tag{3.57}$$

Note that $\langle (v,0)|\psi\rangle = \langle (v,m)|\psi\rangle = \beta = \langle v|\phi\rangle$, and thus the eigenvalue equation is satisfied at all vertices in S with energy $2\cos(k)$. As the eigenstates along a path with energy $2\cos(k)$ are scalar multiples of $\sin(kx)$ and $\cos(kj)$, we can also see that the eigenvalue equation is necessarily satisfied for all (v,j) with $j \neq 0$ and $j \neq m$.

If we then examine the eigenvalue equation at $(v,0)$, we can see that

$$\begin{aligned} \sum_{s \in S_1} \langle s|\psi\rangle + \langle (v,1)|\psi\rangle &= \alpha + \beta\cos(k) + \frac{\gamma - \beta\cos(k)}{\sin(k)}\sin(k) && (3.58) \\ &= \alpha + \gamma && (3.59) \\ &= 2\cos(k)\beta = 2\cos(k)\langle (v,0)|\psi\rangle && (3.60) \end{aligned}$$

where the third equality follows from the fact that $|\phi\rangle$ satisfies the eigenvalue equation at v with eigenvalue $2\cos(k)$.

Let us finally examine the eigenvalue equation at (v,m), noting that

$$\begin{aligned} \sum_{s \in S_2} \langle s|\psi\rangle + \langle (v,m-1)|\psi\rangle &= \gamma + \beta\cos(k(m-1)) + \frac{\gamma - \beta\cos(k)}{\sin(k)}\sin(k(m-1)) && (3.61) \\ &= \gamma + \beta\cos(k) - \big(\gamma - \beta\cos(k)\big) && (3.62) \\ &= 2\cos(k)\beta = 2\cos(k)\langle (v,0)|\psi\rangle && (3.63) \end{aligned}$$

where the second equality follows from some trigonometric identities. We can then see that $|\psi\rangle$ satisfies the eigenvalue equation at (v, m) with energy $2\cos(k)$.

Putting this together, we have that $|\psi\rangle$ is an eigenvector of $A(H)$ with energy $2\cos(k)$ such that $|\psi\rangle$ and $|\phi\rangle$ are identical on those vertices contained in both G and H. As this result holds for any energy $2\cos(k)$ eigenvector of $A(G)$, and as the two graphs are identical along the semi-inifinite paths, we have that the scattering matrices for these two graphs are identical, and thus the scattering matrices are preserved under this degree reduction procedure. $\square$

By repeated use of this lemma, we can then see that if we are only interested in the scattering behavior of a graph at particular momenta, then we need only examine degree three graphs.

3.5.2 Not all momenta can be split

In addition, it might be useful to see when particular scattering behavior is possible or not. As such ,we will show that no momentum switch can exist between the pairs of momenta $-\frac{\pi}{4}$ and $-\frac{3\pi}{4}$. The proof will actually show that no R/T gadget exists between these two momenta, but as any momentum switch can be turned into an R/T gadget, this will be sufficient.

[**TO DO:** *Go over this section, and revise*]

3.5.2.1 Basis vectors with entries in $\mathbb{Q}(\sqrt{2})$

Recall the general setup shown in Figure **??**: N semi-infinite paths are attached to a finite graph $\hat{G}$. Consider an eigenvector $|\tau_k\rangle$ of the adjacency matrix of G with eigenvalue $2\cos(k)$ for $k \in (-\pi, 0)$. In general this eigenspace is spanned by incoming scattering states with momentum k and confined bound states [**?**] (which have zero amplitude on the semi-infinite paths). We can thus write the amplitudes of $|\tau_k\rangle$ on the semi-infinite paths as

$$\langle (x,j)|\tau_k\rangle = \kappa_j \cos(k(x-1)) + \sigma_j \sin(k(x-1))$$

for $x \in \mathbb{Z}^+$, $j \in [N]$, and $\kappa_j, \sigma_j \in \mathbb{C}$, and the amplitudes on the internal vertices as

$$\langle w|\tau_k\rangle = \iota_w$$

for $\iota_w \in \mathbb{C}$, where w indexes the internal vertices. We write the adjacency matrix of $\hat{G}$ as a block matrix as in (**??**). Since the state $|\tau_k\rangle$ satisfies the eigenvalue equation on the semi-infinite paths, it remains to satisfy the conditions specified by the block matrix equation

$$\begin{pmatrix} A & B^\dagger \\ B & D \end{pmatrix}\begin{pmatrix} \kappa \\ \iota \end{pmatrix} + \cos(k)\begin{pmatrix} \kappa \\ 0 \end{pmatrix} + \sin(k)\begin{pmatrix} \sigma \\ 0 \end{pmatrix} = 2\cos(k)\begin{pmatrix} \kappa \\ \iota \end{pmatrix}.$$

Hence, the nullspace of the matrix

$$M = \begin{pmatrix} A - \cos(k)\mathbb{I} & \sin(k)\mathbb{I} & B^\dagger \\ 0 & 0 & 0 \\ B & 0 & D - 2\cos(k)\mathbb{I} \end{pmatrix}$$

is in one-to-one correspondence with the $2\cos(k)$-eigenspace of the infinite matrix (here the first block corresponds to κ, the second to σ, and the third to ι). Further, M only has entries in $\mathbb{Q}(\cos(k), \sin(k))$, so its nullspace has a basis with amplitudes in $\mathbb{Q}(\cos(k), \sin(k))$, as can be seen using Gaussian elimination.

We are interested in the specific cases $2\cos(k) = \pm\sqrt{2}$ corresponding to $k = -\frac{\pi}{4}$ or $k = -\frac{3\pi}{4}$. In these cases $\mathbb{Q}(\cos(k), \sin(k)) = \mathbb{Q}(\sqrt{2})$, and we may choose a basis for the nullspace of M with amplitudes from $\mathbb{Q}(\sqrt{2})$. Furthermore, $\cos(kx), \sin(kx) \in \mathbb{Q}(\sqrt{2})$ for all $x \in \mathbb{Z}^+$, so with such a choice of basis, each amplitude of $|\tau_k\rangle$ is also an element of $\mathbb{Q}(\sqrt{2})$.

As noted above, the spectrum of G may include confined bound states [**?**] with eigenvalue $\pm\sqrt{2}$. However, any such states are eigenstates of the adjacency matrix of $\hat{G}$ subject to the additional (rational) constraints that the amplitudes on the terminals are zero. As such, the confined bound states have a basis over $\mathbb{Q}(\sqrt{2})$. We can use this basis to restrict attention to those states orthogonal to confined bound states using only constraints over $\mathbb{Q}(\sqrt{2})$, so there exists a basis over $\mathbb{Q}(\sqrt{2})$ for the N-dimensional subspace of scattering states with energy $\pm\sqrt{2}$ that are orthogonal to the confined bound states. Finally, since $\mathbb{Q}(\sqrt{2})$ can be seen as a two-dimensional vector space over $\mathbb{Q}$, note that for any member of this basis $|\tau_k\rangle$ there exist rational vectors $|u_k\rangle, |w_k\rangle$ such that $|\tau_k\rangle = |u_k\rangle + \sqrt{2}|w_k\rangle$. Since $H^2|\tau_k\rangle = 2|\tau_k\rangle$, we have $H|u_k\rangle = \pm 2|w_k\rangle$ and $H|w_k\rangle = \pm|u_k\rangle$, so

$$|\tau_k\rangle = (H \pm \sqrt{2}\mathbb{I})|w_k\rangle. \tag{3.64}$$

3.5.2.2 No R/T gadget and hence no momentum switch

Recall from Section **??** that a momentum switch between two momenta k and p can always be converted into an R/T gadget between k and p. Here we show that if an R/T gadget perfectly reflects at momentum $-\frac{\pi}{4}$, then it must also perfectly reflect at momentum $-\frac{3\pi}{4}$. This implies that no R/T gadget exists between these two momenta, and thus no momentum switch exists.

We use the following basic fact about two-terminal gadgets several times:

Fact 1. *If a two-terminal gadget has a momentum-k scattering state $|\phi\rangle$ with zero amplitude along path 2, then the gadget perfectly reflects at momentum k.*

Proof. Without loss of generality, we may assume that $|\phi\rangle$ is orthogonal to all confined bound states. If $|\phi\rangle$ has zero amplitude along path 2, then there exist some $\mu, \nu \in \mathbb{C}$ such that

$$\langle (x,2)|\phi\rangle = \mu\langle (x,2)|{}_2(k)\rangle + \nu\langle (x,2)|{}_1(k)\rangle = \mu e^{-ikx} + \mu R e^{ikx} + \nu T e^{ikx} = 0$$

for all $x \in \mathbb{Z}^+$. Since this holds for all x, we have $\mu = \mu R + \nu T = 0$. Since μ and ν cannot both be zero, we have $T = 0$. $\square$

For an R/T gadget, the scattering states (at some fixed momentum) that are orthogonal to the confined bound states span a two-dimensional space. As shown in Section 3.5.2.1, we can expand each scattering eigenstate at momentum $k = -\frac{\pi}{4}$ in a basis with entries in $\mathbb{Q}(\sqrt{2})$, where each basis vector takes the form (3.64). This gives

$$|{}_1(-\tfrac{\pi}{4})\rangle = (H + \sqrt{2}\mathbb{I})(\alpha|\Game\rangle + \beta|\ \rangle)$$

where $\alpha, \beta \in \mathbb{C}$, $\alpha \neq 0$, and $|\, a\,\rangle$ and $|\, b\,\rangle$ are rational 2-eigenvectors of H^2.

If $T(-\frac{\pi}{4}) = 0$, then for all $x \geq 0$,

$$\langle x, 2|\,{}_1(-\tfrac{\pi}{4})\,\rangle = 0 = \langle x, 2|(H + \sqrt{2}\mathbb{I})(\alpha|\ni\rangle + \beta|\ \rangle).$$

Dividing through by α and rearranging, we get that for all $x \geq 0$,

$$\frac{\beta}{\alpha}(\langle x, 2|H|\,b\,\rangle + \sqrt{2}\langle x, 2|\,b\,\rangle) = -\langle x, 2|H|\,a\,\rangle - \sqrt{2}\langle x, 2|\,a\,\rangle.$$

If the left-hand side is not zero, then $\beta/\alpha \in \mathbb{Q}(\sqrt{2})$ since H, $|\,a\,\rangle$, and $|\,b\,\rangle$ are rational. If the left-hand side is zero, then $(H + \sqrt{2}\mathbb{I})|\,a\,\rangle$ is an eigenstate at energy $2\cos(k)$ with no amplitude along path 2, so $\beta = 0$ (using Fact 1), and again $\beta/\alpha \in \mathbb{Q}(\sqrt{2})$.

Now write $\beta/\alpha = r + s\sqrt{2}$ with $r, s \in \mathbb{Q}$, and consider the rational 2-eigenvector of H^2

$$|\,c\,\rangle := |\,a\,\rangle + (r + sH)|\,b\,\rangle.$$

Note that

$$\alpha(H + \sqrt{2}\mathbb{I})|\,c\,\rangle = \alpha(H + \sqrt{2}\mathbb{I})|\,a\,\rangle + \alpha(rH + r\sqrt{2} + sH^2 + sH\sqrt{2})|\,b\,\rangle.$$

Since $|\,b\,\rangle$ is a 2-eigenvector of H^2 and $\beta/\alpha = r + s\sqrt{2}$, this simplifies to

$$\alpha(H + \sqrt{2}\mathbb{I})|\,c\,\rangle = \alpha(H + \sqrt{2}\mathbb{I})|\,a\,\rangle + \beta(H + \sqrt{2}\mathbb{I})|\,b\,\rangle = |\,{}_1(-\tfrac{\pi}{4})\,\rangle, \tag{3.65}$$

so $|\,{}_1(-\frac{\pi}{4})\,\rangle$ can be written as $\alpha(H + \sqrt{2}\mathbb{I})$ times a rational 2-eigenvector of H^2.

Since $\langle x, 2|\,{}_1(-\frac{\pi}{4})\,\rangle = 0$ for all $x \geq 1$ (and $\alpha \neq 0$), we have

$$\langle x, 2|(H + \sqrt{2}\mathbb{I})|\,c\,\rangle = \langle x, 2|H|\,c\,\rangle + \sqrt{2}\langle x, 2|\,c\,\rangle = 0.$$

As H is a rational matrix and $|\,c\,\rangle$ is a rational vector, the rational and irrational components must both be zero, implying $\langle x, 2|\,c\,\rangle = \langle x, 2|H|\,c\,\rangle = 0$ for all $x \geq 1$. Furthermore, since $|\,{}_1(-\frac{\pi}{4})\,\rangle$ is a scattering state with zero amplitude on path 2, it must have some nonzero amplitude on path 1 and thus there is some $x_0 \in \mathbb{Z}^+$ for which $\langle x_0, 1|\,c\,\rangle \neq 0$ or $\langle x_0, 1|H|\,c\,\rangle \neq 0$.

Now consider the state obtained by replacing $\sqrt{2}$ with $-\sqrt{2}$:

$$|\,{}_1(-\tfrac{\pi}{4})\,\rangle := \alpha(H - \sqrt{2}\mathbb{I})|\,c\,\rangle.$$

This is a $-\sqrt{2}$-eigenvector of H, which can be confirmed using the fact that $|\,c\,\rangle$ is a 2-eigenvector of H^2. As $\langle x, 2|H|c\rangle = \langle x, 2|c\rangle = 0$ for all $x \geq 1$, $\langle x, 2|\,{}_1(-\frac{\pi}{4})\,\rangle = 0$ for all $x \geq 1$. Furthermore the amplitude at vertex $(x_0, 1)$ is nonzero, i.e., $\langle x_0, 1|\,{}_1(-\frac{\pi}{4})\,\rangle \neq 0$, and hence $|\,{}_1(-\frac{\pi}{4})\,\rangle$ has a component orthogonal to the space of confined bound states (which have zero amplitude on both semi-infinite paths). Hence, there exists a scattering state with eigenvalue $-\sqrt{2}$ with no amplitude on path 2. By Fact 1, the gadget perfectly reflects at momentum $-\frac{3\pi}{4}$. It follows that no perfect R/T gadget (and hence no perfect momentum switch) exists between these momenta.

This proof technique can also establish non-existence of momentum switches between other pairs of momenta k and p. For example, a slight modification of the above proof shows that no momentum switch exists between $k = -\frac{\pi}{6}$ and $p = -\frac{5\pi}{6}$.

3.5.3 Laplacians vs adjacency matrix

[**TO DO:** *If I have time, write this section*]

3.6 Conclusions and open problems

I need to say something here.

Find more gates.

Determine necessary conditions for momentum switches to occur.

Basically just do more research.

Chapter 4

Universality of single-particle scattering

4.1 Finite truncation

I think I should include theorem 1 here (maybe)

Theorem 1. *Let $\widehat{G}$ be an $(N+m)$-vertex graph. Let G be the graph obtained from $\widetilde{G}$ by attaching semi-infinite paths to the first N of its vertices, and let S be the corresponding S-matrix. Let H_G be the quantum walk Hamiltonian of equation [**CITE:** correct equation] . Let $k \in (-\pi, 0)$, $M, L \in \mathbb{N}$, $j \in [N]$, and*

$$|\,\psi^j(0)\,\rangle = \frac{1}{\sqrt{L}} \sum_{x=M+1}^{M4L} e^{-ikx} |\,x, j\,\rangle. \tag{4.1}$$

Let c_0 be a constant independent of L. Then, for all $0 \le t \le c_0 L$,

$$\left\| e^{-iH_G t} |\,\psi^j(0)\,\rangle - |\,\alpha^j(t)\,\rangle \right\| = \mathcal{O}(L^{-1/4}) \tag{4.2}$$

where

$$|\,\alpha^j(t)\,\rangle = \frac{1}{\sqrt{L}} e^{-2it\cos k} \sum_{x=1}^{\infty} \sum_{q=1}^{N} (\delta_{qj} e^{-ikx} R(x - \lfloor 2t \sin k \rfloor) + S_{qj}(k) e^{ikx} R(-x - \lfloor 2t \sin k \rfloor)) |\,x, q\,\rangle \tag{4.3}$$

with

$$R(l) = \begin{cases} 1 & \text{if } l - M \in [L] \\ 0 & \text{otherwise.} \end{cases} \tag{4.4}$$

n this section we prove Theorem **??**. The proof is based on (and follows closely) the calculation from the appendix of reference [**?**].

Recall from (**??**) that the scattering eigenstates of $H_G^{(1)}$ have the form

$$\langle x, q | \mathrm{sc}_j(k) \rangle = e^{-ikx} \delta_{qj} + e^{ikx} S_{qj}(k)$$

for each $k \in (-\pi, 0)$.

Before delving into the proof, we first establish that the state $|\alpha^j(t)\rangle$ is approximately normalized. This state is not normalized at all times t. However, $\langle\alpha^j(t)|\alpha^j(t)\rangle = 1+\mathcal{O}(L^{-1})$, as we now show:

$$\begin{aligned}
\langle\alpha^j(t)|\alpha^j(t)\rangle &= \frac{1}{L}\sum_{x=1}^{\infty}\left|e^{-ikx}R(x-\lfloor 2t\sin k\rfloor)+S_{jj}(k)e^{ikx}R(-x-\lfloor 2t\sin k\rfloor)\right|^2\\
&\quad+\frac{1}{L}\sum_{q\neq j}\sum_{x=1}^{\infty}|S_{qj}(k)|^2R(-x-\lfloor 2t\sin k\rfloor)\\
&=\frac{1}{L}\sum_{x=1}^{\infty}\left[R(x-\lfloor 2t\sin k\rfloor)+R(-x-\lfloor 2t\sin k\rfloor)\right]\\
&\quad+\frac{1}{L}\sum_{x=1}^{\infty}\left(e^{-2ikx}S^*_{jj}(k)+e^{2ikx}S_{jj}(k)\right)R(x-\lfloor 2t\sin k\rfloor)R(-x-\lfloor 2t\sin k\rfloor)\\
&=1+\frac{1}{L}\sum_{x=1}^{\infty}\left(e^{-2ikx}S^*_{jj}(k)+e^{2ikx}S_{jj}(k)\right)R(x-\lfloor 2t\sin k\rfloor)R(-x-\lfloor 2t\sin k\rfloor)+\mathcal{O}(L^{-1})
\end{aligned}$$

where we have used unitarity of S in the second step. When it is nonzero, the second term can be written as

$$\frac{1}{L}\sum_{x=1}^{b}\left(e^{-2ikx}S^*_{jj}(k)+e^{2ikx}S_{jj}(k)\right)$$

where b is the maximum positive integer such that $\{-b,b\}\subset\{M+1+\lfloor 2t\sin k\rfloor,\ldots,M+L+\lfloor 2t\sin k\rfloor\}$. Performing the sums, we get

$$\begin{aligned}
\left|\frac{1}{L}\sum_{x=1}^{b}\left(e^{-2ikx}S^*_{jj}(k)+e^{2ikx}S_{jj}(k)\right)\right| &= \frac{1}{L}\left|S^*_{jj}(k)e^{-2ik}\frac{e^{-2ikb}-1}{e^{-2ik}-1}+S_{jj}(k)e^{2ik}\frac{e^{2ikb}-1}{e^{2ik}-1}\right|\\
&\le\frac{2}{L|\sin k|}.
\end{aligned}$$

Thus we have $\langle\alpha^j(t)|\alpha^j(t)\rangle = 1+\mathcal{O}(L^{-1})$.

Proof of Theorem **??**. Define

$$|\psi^j(t)\rangle = e^{-iH_G^{(1)}t}|\psi^j(0)\rangle$$

and write

$$|\psi^j(t)\rangle = |w^j(t)\rangle + |v^j(t)\rangle$$

where

$$|w^j(t)\rangle = \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}e^{-2it\cos(k+\phi)}\sum_{q=1}^{N}|\mathrm{sc}_q(k+\phi)\rangle\langle\mathrm{sc}_q(k+\phi)|\psi^j(0)\rangle$$

and $\langle w^j(t)|v^j(t)\rangle = 0$. We take $\epsilon = \frac{|\sin k|}{2\sqrt{L}}$. Now

$$\langle\mathrm{sc}_q(k+\phi)|\psi^j(0)\rangle = \frac{1}{\sqrt{L}}\sum_{x=M+1}^{M+L}\left(e^{i\phi x}\delta_{qj}+e^{-i(2k+\phi)x}S^*_{qj}(k+\phi)\right),$$

so

$$|w^j(t)\rangle = |w_A^j(t)\rangle + \sum_{q=1}^{N} |w_B^{q,j}(t)\rangle$$

where

$$\begin{aligned}
|w_A^j(t)\rangle &= \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} e^{-2it\cos(k+\phi)} f(\phi) |\mathrm{sc}_j(k+\phi)\rangle \\
|w_B^{q,j}(t)\rangle &= \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} e^{-2it\cos(k+\phi)} g_{qj}(\phi) |\mathrm{sc}_q(k+\phi)\rangle
\end{aligned}$$

with

$$\begin{aligned}
f(\phi) &= \frac{1}{\sqrt{L}} \sum_{x=M+1}^{M+L} e^{i\phi x} \\
g_{qj}(\phi) &= \frac{1}{\sqrt{L}} \sum_{x=M+1}^{M+L} e^{-i(2k+\phi)x} S_{qj}^*(k+\phi).
\end{aligned}$$

We will see that $|\,\psi^j(t)\,\rangle \approx |\,w^j(t)\,\rangle \approx |\,w_A^j(t)\,\rangle \approx |\,\alpha^j(t)\,\rangle$.

Now

$$\langle w_A^j(t)|w_A^j(t)\rangle = \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} |f(\phi)|^2 = \frac{1}{L}\int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)}$$

but

$$\frac{1}{L}\int_{-\pi}^{\pi} \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)} = 1$$

and

$$\begin{aligned}
\frac{1}{L}\left(\int_{\epsilon}^{\pi} + \int_{-\pi}^{-\epsilon}\right) \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)} &= \frac{2}{L}\int_{\epsilon}^{\pi} \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)} \\
&\le \frac{2}{L}\int_{\epsilon}^{\pi} \frac{d\phi}{2\pi} \frac{\pi^2}{\phi^2} \\
&\le \frac{\pi}{L\epsilon}. \qquad (4.5)
\end{aligned}$$

Therefore

$$1 \ge \langle w_A^j(t)|w_A^j(t)\rangle \ge 1 - \frac{\pi}{L\epsilon}.$$

Similarly,

$$\langle w_B^{qj}(t)|w_B^{qj}(t)\rangle = \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \frac{|S_{qj}(k+\phi)|^2}{L} \frac{\sin^2(\frac{1}{2}L(2k+\phi))}{\sin^2(\frac{1}{2}(2k+\phi))},$$

and, using the unitarity of S,

$$\begin{aligned}
\sum_{q=1}^{N} \langle w_B^{qj}(t)|w_B^{qj}(t)\rangle &= \frac{1}{L}\int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L(2k+\phi))}{\sin^2(\frac{1}{2}(2k+\phi))} \\
&\le \frac{1}{L}\int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \frac{1}{\sin^2(\frac{1}{2}(2k+\phi))}.
\end{aligned}$$

Now $|\sin(k+\phi/2)-\sin k| \le |\phi|/2$ (by the mean value theorem). So

$$\sin^2\left(k+\frac{\phi}{2}\right) \ge \left(|\sin k| - \left|\frac{\phi}{2}\right|\right)^2.$$

Since $\epsilon = \frac{|\sin k|}{2\sqrt{L}} < |\sin k|$ we then have

$$\begin{aligned}\sum_{q=1}^{N}\langle w_B^{qj}(t)|w_B^{qj}(t)\rangle &\le \frac{1}{L}\int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\frac{4}{\sin^2 k}\\ &= \frac{4\epsilon}{\pi L\sin^2 k}.\end{aligned}$$

Hence

$$\begin{aligned}\langle w^j(t)|w^j(t)\rangle &\ge \langle w_A^j(t)|w_A^j(t)\rangle - 2\left|\sum_{q=1}^{N}\langle w_A^j(t)|w_B^{qj}(t)\rangle\right|\\ &\ge 1-\frac{\pi}{L\epsilon} - 2\left\|\sum_{q=1}^{n}|w_B^{qj}(t)\rangle\right\|\\ &\ge 1-\frac{\pi}{L\epsilon} - 2\sum_{q=1}^{n}\left\||w_B^{qj}(t)\rangle\right\|\\ &\ge 1-\frac{\pi}{L\epsilon} - 4\sqrt{\frac{\epsilon N}{\pi L\sin^2 k}},\end{aligned}$$

so

$$\langle v^j(t)|v^j(t)\rangle \le \frac{\pi}{L\epsilon} + 4\sqrt{\frac{\epsilon N}{\pi L\sin^2 k}}$$

since $\langle v^j(t)|v^j(t)\rangle + \langle w^j(t)|w^j(t)\rangle = 1$. Thus

$$\begin{aligned}\left\||\psi^j(t)\rangle - |w_A^j(t)\rangle\right\| &= \left\||v^j(t)\rangle + \sum_{q=1}^{N}|w_B^{qj}(t)\rangle\right\|\\ &\le \left(\frac{\pi}{L\epsilon} + 4\sqrt{\frac{\epsilon N}{\pi L\sin^2 k}}\right)^{\frac{1}{2}} + 2\sqrt{\frac{\epsilon N}{\pi L\sin^2 k}}.\end{aligned}$$

With our choice $\epsilon = \frac{|\sin k|}{2\sqrt{L}}$, we have $\left\||\psi^j(t)\rangle - |w_A^j(t)\rangle\right\| = \emptyset(L^{-1/4})$.

We now show that

$$\left\||w_A^j(t)\rangle - |\alpha^j(t)\rangle\right\| = \emptyset(L^{-1/8}). \tag{4.6}$$

Letting

$$P = \sum_{q=1}^{N}\sum_{x=1}^{\infty}|x,q\rangle\langle x,q|$$

be the projector onto the semi-infinite paths, to show equation (4.6) it is sufficient to show that

$$\left\| P|w_A^j(t)\rangle - |\alpha^j(t)\rangle \right\| = \emptyset(L^{-1/4}) \tag{4.7}$$

since this implies that

$$\begin{aligned}\left\| P|w_A^j(t)\rangle \right\| &= \left\| |\alpha^j(t)\rangle \right\| + \emptyset(L^{-1/4}) \\ &= 1 + \emptyset(L^{-1/4})\end{aligned}$$

and hence

$$\begin{aligned}\left\| (1-P)\,|w_A^j(t)\rangle \right\|^2 &= \left\| |w_A^j(t)\rangle \right\|^2 - \left\| P|w_A^j(t)\rangle \right\|^2 \\ &\leq 1 - \left(1 + \emptyset(L^{-1/4})\right) \\ &= \emptyset(L^{-1/4}).\end{aligned} \tag{4.8}$$

From the above formula we now see that inequality (4.7) implies (4.6).

Noting that

$$\frac{1}{\sqrt{L}} R(l) = \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi l} f(\phi),$$

we write

$$\begin{aligned}\langle x, q|\alpha^j(t)\rangle = e^{-2it\cos k} \Bigg(&\delta_{qj} e^{-ikx} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi(x - \lfloor 2t\sin k \rfloor)} f(\phi) \\ &+ S_{qj}(k) e^{ikx} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi(-x - \lfloor 2t\sin k \rfloor)} f(\phi) \Bigg).\end{aligned} \tag{4.9}$$

On the other hand,

$$\langle x, q|w_A^j(t)\rangle = \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} e^{-2it\cos(k+\phi)} f(\phi) \left(e^{-i(k+\phi)x} \delta_{qj} + e^{i(k+\phi)x} S_{qj}(k+\phi) \right). \tag{4.10}$$

Using equations (4.9) and (4.10) we can write

$$P|w_A^j(t)\rangle = |\alpha^j(t)\rangle + \sum_{i=1}^{7} |c_i^j(t)\rangle$$

where $P|c_i^j(t)\rangle = |c_i^j(t)\rangle$ and

$$\begin{aligned}
\langle x, q|c_1^j(t)\rangle &= \delta_{qj} e^{-2it\cos k} e^{-ikx} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi x} f(\phi) \left(e^{2it\phi\sin k} - e^{i\phi\lfloor 2t\sin k\rfloor}\right) \\
\langle x, q|c_2^j(t)\rangle &= S_{qj}(k) e^{-2it\cos k} e^{ikx} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{i\phi x} f(\phi) \left(e^{2it\phi\sin k} - e^{i\phi\lfloor 2t\sin k\rfloor}\right) \\
\langle x, q|c_3^j(t)\rangle &= -\delta_{qj} e^{-2it\cos k} e^{-ikx} \left(\int_{\epsilon}^{\pi} + \int_{-\pi}^{-\epsilon}\right) \frac{d\phi}{2\pi} e^{-i\phi x} f(\phi) e^{2it\phi\sin k} \\
\langle x, q|c_4^j(t)\rangle &= -S_{qj}(k) e^{-2it\cos k} e^{ikx} \left(\int_{\epsilon}^{\pi} + \int_{-\pi}^{-\epsilon}\right) \frac{d\phi}{2\pi} e^{i\phi x} f(\phi) e^{2it\phi\sin k} \\
\langle x, q|c_5^j(t)\rangle &= \delta_{qj} e^{-ikx} \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} e^{-i\phi x} f(\phi) \left(e^{-2it\cos(k+\phi)} - e^{-2it\cos k + 2it\phi\sin k}\right) \\
\langle x, q|c_6^j(t)\rangle &= S_{qj}(k) e^{ikx} \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} e^{i\phi x} f(\phi) \left(e^{-2it\cos(k+\phi)} - e^{-2it\cos k + 2it\phi\sin k}\right) \\
\langle x, q|c_7^j(t)\rangle &= e^{ikx} \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} e^{i\phi x} e^{-2it\cos(k+\phi)} f(\phi) \left(S_{qj}(k+\phi) - S_{qj}(k)\right).
\end{aligned}$$

We now bound the norm of each of these states:

$$\begin{aligned}
\langle c_1^j(t)|c_1^j(t)\rangle &= \sum_{q=1}^{N} \sum_{x=1}^{\infty} \left| \delta_{qj} e^{-2it\cos k} e^{-ikx} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi x} f(\phi) \left(e^{2it\phi\sin k} - e^{i\phi\lfloor 2t\sin k\rfloor}\right) \right|^2 \\
&\le \sum_{q=1}^{N} \sum_{x=-\infty}^{\infty} \left| \delta_{qj} e^{-2it\cos k} e^{-ikx} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi x} f(\phi) \left(e^{2it\phi\sin k} - e^{i\phi\lfloor 2t\sin k\rfloor}\right) \right|^2 \\
&= \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} |f(\phi)|^2 \left|e^{2it\phi\sin k} - e^{i\phi\lfloor 2t\sin k\rfloor}\right|^2 \\
&\le \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} |f(\phi)|^2 \left(2t\phi\sin k - \lfloor 2t\sin k\rfloor \phi\right)^2 \\
&\le \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} |f(\phi)|^2 \phi^2
\end{aligned}$$

where we have used the facts that $|e^{is} - 1|^2 \le s^2$ for $s \in \mathbb{R}$ and $|2t\sin k - \lfloor 2t\sin k\rfloor| < 1$. In the above we performed the sum over x using the identity

$$\sum_{x=-\infty}^{\infty} e^{i(\phi - \tilde{\phi})x} = 2\pi\delta(\phi - \tilde{\phi}) \text{ for } \phi, \tilde{\phi} \in (-\pi, \pi).$$

We use this fact repeatedly in the following calculations. Continuing, we get

$$\begin{aligned}
\langle c_1^j(t)|c_1^j(t)\rangle &\le \frac{1}{L} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)} \phi^2 \\
&\le \frac{1}{L} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} \frac{1}{\sin^2(\frac{1}{2}\phi)} \phi^2 \\
&\le \frac{\pi^2}{L}
\end{aligned}$$

using the fact that $\sin^2(\phi/2) \geq \phi^2/\pi^2$ for $\phi \in [-\pi, \pi]$. Similarly we bound $\langle c_2^j(t)|c_2^j(t)\rangle \leq \pi^2/L$.

Using equation (4.5) we get

$$\begin{aligned}\langle c_3^j(t)|c_3^j(t)\rangle &\leq \left(\int_{\epsilon}^{\pi} + \int_{-\pi}^{-\epsilon}\right)\frac{d\phi}{2\pi}\left|f(\phi)\right|^2 \\ &\leq \frac{\pi}{L\epsilon}\end{aligned}$$

and similarly for $\langle c_4^j(t)|c_4^j(t)\rangle$. Next, we have

$$\begin{aligned}\langle c_5^j(t)|c_5^j(t)\rangle &\leq \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\left|e^{-2it\cos(k+\phi)} - e^{-2it\cos k + 2it\phi\sin k}\right|^2 \\ &\leq \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\left(2t\cos\left(k+\phi\right) - 2t\cos k + 2t\phi\sin k\right)^2 \\ &= \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\left(2t\cos k\left(\cos\phi - 1\right) + 2t\sin k\left(\phi - \sin\phi\right)\right)^2 \\ &\leq \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2 4t^2\phi^4 \\ &= \frac{4t^2}{L}\int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)}\phi^4 \\ &\leq \frac{4t^2}{L}\int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\pi^2\phi^2 \\ &= \frac{4\pi}{3L}t^2\epsilon^3\end{aligned}$$

and we have the same bound for $|c_6^j(t)\rangle$. Finally,

$$\langle c_7^j(t)|c_7^j(t)\rangle \leq \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\sum_{q=1}^{N}\left|S_{qj}(k+\phi) - S_{qj}(k)\right|^2.$$

Now, for each $q \in \{1, \ldots, N\}$,

$$|S_{qj}(k+\phi) - S_{qj}(k)| \leq \Gamma|\phi|$$

where the Lipschitz constant

$$\Gamma = \max_{q,j\in\{1,\ldots,N\}}\max_{k'\in[-\pi,\pi]}\left|\frac{d}{dk'}S_{qj}(k')\right|$$

is well defined since each matrix element $S_{qj}(k')$ is a bounded rational function of $e^{ik'}$, as can be seen from equation (**??**). Hence

$$\begin{aligned}
\langle c_7^j(t)|c_7^j(t)\rangle &\leq \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \left|f(\phi)\right|^2 N\Gamma^2\phi^2 \\
&= \frac{N\Gamma^2}{L}\int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi}\frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)}\phi^2 \\
&\leq \frac{N\Gamma^2}{L}\int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi}\pi^2 \\
&= N\Gamma^2\frac{\pi\epsilon}{L}.
\end{aligned}$$

Now using the bounds on the norms of each of these states we get

$$\begin{aligned}
\big\|P|w_A^j(t)\rangle - |\alpha^j(t)\rangle\big\| &\leq 2\frac{\pi}{\sqrt{L}} + 2\sqrt{\frac{\pi}{L\epsilon}} + 2\sqrt{\frac{4\pi}{3L}t^2\epsilon^3} + \sqrt{N\Gamma^2\frac{\pi\epsilon}{L}} \\
&= \emptyset(L^{-1/4})
\end{aligned}$$

using the choice $\epsilon = \frac{|\sin p|}{2\sqrt{L}}$ and the fact that $t = \emptyset(L)$. $\square$

Note that this analysis assumes that $N = \emptyset(1)$, which is the case in our applications of Theorem **??**.

4.2 Using scattering for simple computation

4.3 Encoded two-qubit gates

4.4 Single-qubit blocks

4.5 Combining blocks

It might be worthwhile to include a new proof of universal computation of single-particle scattering in this model.

Chapter 5

Universality of multi-particle scattering

I should really give a broad overview of the technique. Maybe not in any great detail, but I should really explain why things are going to go the way they are.

5.1 Multi-particle quantum walk

Now that we have analyzed the single particle quantum walk, we will want to understand how the multi-particle system works together. Unfortunately, this system is difficult in general to analyze, as the various interactions become intractable. In fact, we will eventually show that this is as hard as understanding the amplitudahedron, also known as universal quantum computation.

5.1.1 Two-particle scattering on an infinite path

While understanding the interactions of multi-particle interactions on an arbitrary graph is beyond our current understanding, we can simplify the model, and see what we can understand. Along those lines, we can restrict ourselves to the case where only two particles interact. Similarly, we can restrict ourselves to understanding their interaction on the most simple infinite graph; namely the infinite path.

As such, let us assume that there is some interaction with finite range between the particles, that depends only on the distance between the particles.

Here we derive scattering states of the two-particle quantum walk on an infinite path. We write the Hamiltonian in the basis $|x,y\rangle$, where x denotes the location of the first particle and y denotes the location of the second particle, with the understanding that bosonic states are symmetrized and fermionic states are antisymmetrized. The Hamiltonian (**??**) can be written as

$$H^{(2)} = H_x^{(1)} \otimes \mathbb{I}_y + \mathbb{I}_x \otimes H_y^{(1)} + \sum_{x,y\in\mathbb{Z}} \mathcal{V}(|x-y|)\,|x,y\rangle\langle x,y| \tag{5.1}$$

where $\mathcal{V}$ corresponds to the interaction term $\mathcal{U}$ and (with a slight abuse of notation) the subscript indicates which variable is acted on. Here

$$H^{(1)} = \sum_{x\in\mathbb{Z}} |\, x+1\,\rangle\langle\, x\,| + |\, x\,\rangle\langle\, x+1\,|$$

is the adjacency matrix of an infinite path. Our assumption that $\mathcal{U}$ has finite range C means that $\mathcal{V}(r) = 0$ for $r > C$.

The scattering states we are interested in provide information about the dynamics of two particles initially prepared in spatially separated wave packets moving toward each other along the path with momenta $k_1 \in (-\pi, 0)$ and $k_2 \in (0, \pi)$.

We derive scattering eigenstates of this Hamiltonian by transforming to the new variables $s = x + y$ and $r = x - y$ and exploiting translation symmetry. Here the allowed values (s, r) range over the pairs of integers where either both are even or both are odd. Writing states in this basis as $|s; r\rangle$, the Hamiltonian takes the form

$$H_s^{(1)} \otimes H_r^{(1)} + \mathbb{I}_s \otimes \sum_{r\in\mathbb{Z}} \mathcal{V}(|r|)\,|\, r\,\rangle\langle\, r\,|. \tag{5.2}$$

For each $p_1 \in (-\pi, \pi)$ and $p_2 \in (0, \pi)$ there is a scattering eigenstate $|\mathrm{sc}(p_1; p_2)\rangle$ of the form

$$\langle s; r|\mathrm{sc}(p_1; p_2)\rangle = e^{-ip_1 s/2}\langle r|\psi(p_1; p_2)\rangle,$$

where the state $|\psi(p_1; p_2)\rangle$ can be viewed as an effective single-particle scattering state of the Hamiltonian

$$2\cos\left(\frac{p_1}{2}\right) H_r^{(1)} + \sum_{r\in\mathbb{Z}} \mathcal{V}(|r|)\,|\, r\,\rangle\langle\, r\,| \tag{5.3}$$

with eigenvalue $4\cos(p_1/2)\cos(p_2)$. For a given $\mathcal{V}$, the state $|\psi(p_1; p_2)\rangle$ can be obtained explicitly by solving a set of linear equations (see for example [**?**]). It has the form

$$\langle r|\psi(p_1; p_2)\rangle = \begin{cases} e^{-ip_2 r} + R(p_1, p_2)e^{ip_2 r} & \text{if } r \le -C \\ f(p_1, p_2, r) & \text{if } |r| < C \\ T(p_1, p_2)e^{-ip_2 r} & \text{if } r \ge C \end{cases} \tag{5.4}$$

for $p_2 \in (0, \pi)$. Here the reflection and transmission coefficients R and T and the amplitudes of the scattering state for $|r| < C$ (described by the function f) depend on both momenta as well as the interaction $\mathcal{V}$. With R, T, and f chosen appropriately, the state $|\mathrm{sc}(p_1; p_2)\rangle$ is an eigenstate of $H^{(2)}$ with eigenvalue $4\cos(p_1/2)\cos(p_2)$.

Since $\mathcal{V}(|r|)$ is an even function of r, we can also define scattering states for $p_2 \in (-\pi, 0)$ by

$$\langle s; r|\mathrm{sc}(p_1; p_2)\rangle = \langle s; -r|\mathrm{sc}(p_1; -p_2)\rangle.$$

These other states are obtained by swapping x and y, corresponding to interchanging the two particles.

The states $\{|\mathrm{sc}(p_1; p_2)\rangle : p_1 \in (-\pi, \pi),\ p_2 \in (-\pi, 0) \cup (0, \pi)\}$ are (delta-function) orthonormal:

$$\begin{aligned}
\langle \mathrm{sc}(p_1'; p_2') | \mathrm{sc}(p_1; p_2)\rangle &= \langle \mathrm{sc}(p_1'; p_2')| \left(\sum_{r,\, s \text{ even}} |r\rangle\langle r| \otimes |s\rangle\langle s| \right) |\mathrm{sc}(p_1; p_2)\rangle \\
&\quad + \langle \mathrm{sc}(p_1'; p_2')| \left(\sum_{r,\, s \text{ odd}} |r\rangle\langle r| \otimes |s\rangle\langle s| \right) |\mathrm{sc}(p_1; p_2)\rangle \\
&= \sum_{s \text{ even}} e^{-i(p_1 - p_1')s/2} \sum_{r \text{ even}} \langle \psi(p_1'; p_2') | r\rangle \langle r | \psi(p_1; p_2)\rangle \\
&\quad + \sum_{s \text{ odd}} e^{-i(p_1 - p_1')s/2} \sum_{r \text{ odd}} \langle \psi(p_1'; p_2') | r\rangle \langle r | \psi(p_1; p_2)\rangle \\
&= 2\pi\delta(p_1 - p_1') \sum_{r=-\infty}^{\infty} \langle \psi(p_1; p_2') | r\rangle \langle r | \psi(p_1; p_2)\rangle \\
&= 4\pi^2 \delta(p_1 - p_1')\delta(p_2 - p_2')
\end{aligned}$$

where in the last step we used the fact that $\langle \psi(p_1; p_2') | \psi(p_1; p_2)\rangle = 2\pi\delta(p_2 - p_2')$. To construct bosonic or fermionic scattering states, we symmetrize or antisymmetrize as follows. For $p_1 \in (-\pi, \pi)$ and $p_2 \in (0, \pi)$, we define

$$|\,\mathrm{sc}(p_1; p_2)\,\rangle_{\pm} = \frac{1}{\sqrt{2}} (|\,\mathrm{sc}(p_1; p_2)\,\rangle \pm |\,\mathrm{sc}(p_1; -p_2)\,\rangle).$$

Then

$$\langle\, s; r\,|\,\mathrm{sc}(p_1; p_2)\,\rangle_{\pm} = \frac{1}{\sqrt{2}} e^{-ip_1 s/2} \begin{cases} e^{-ip_2 r} \pm e^{i\theta_{\pm}(p_1, p_2)} e^{ip_2 r} & \text{if } r \le -C \\ f(p_1, p_2, r) \pm f(p_1, p_2, -r) & \text{if } |r| < C \\ e^{i\theta_{\pm}(p_1, p_2)} e^{-ip_2 r} \pm e^{ip_2 r} & \text{if } r \ge C \end{cases} \tag{5.5}$$

where $\theta_{\pm}(p_1, p_2)$ is a real function defined through

$$e^{i\theta_{\pm}(p_1, p_2)} = T(p_1, p_2) \pm R(p_1, p_2). \tag{5.6}$$

Note that $|T \pm R| = 1$; this follows from the potential $\mathcal{V}(|r|)$ being even in r and from unitarity of the S-matrix. These eigenstates allow us to understand what happens when two particles with momenta $k_1 \in (-\pi, 0)$ and $k_2 \in (0, \pi)$ move toward each other. Here $p_1 = -k_1 - k_2$ and $p_2 = (k_2 - k_1)/2$. Recall (from the main text of the paper) that we defined $e^{i\theta}$ to be the phase acquired by the two-particle wavefunction when $k_1 = -\pi/2$ and $k_2 = \pi/4$ (θ depends implicitly on the interaction $\mathcal{V}$ and the particle type), so $\theta = \theta_{\pm}(\pi/4, 3\pi/8)$.

For $|r| \ge C$ the scattering state is a sum of two terms, one corresponding to the two particles moving toward each other and one corresponding to the two particles moving apart after scattering. The outgoing term has a phase of $T \pm R$ relative to the incoming term (as depicted in Figure **??**). This phase arises from the interaction between the two particles.

For example, consider the Bose-Hubbard model, where $\mathcal{V}(|r|) = U\delta_{r,0}$. Here $C = 0$ and $T = 1 + R$. In this case the scattering state $|\mathrm{sc}(p_1; p_2)\rangle_+$ is

$$\langle x, y | \mathrm{sc}(p_1; p_2)\rangle_+ = \frac{1}{\sqrt{2}} e^{-ip_1\left(\frac{x+y}{2}\right)} \left(e^{ip_2|x-y|} + e^{i\theta_+(p_1, p_2)} e^{-ip_2|x-y|} \right).$$

The first term describes the two particles moving toward each other and the second term describes them moving away from each other. To solve for the applied phase $e^{i\theta_+(p_1,p_2)}$ we look at the eigenvalue equation for $|\psi(p_1;p_2)\rangle$ at $r=0$. This gives

$$R(p_1,p_2) = -\frac{U}{U-4i\cos(p_1/2)\sin(p_2)}.$$

So for the Bose-Hubbard model,

$$e^{i\theta_+(p_1,p_2)} = T(p_1,p_2)+R(p_1,p_2) = -\frac{U+4i\cos(p_1/2)\sin(p_2)}{U-4i\cos(p_1/2)\sin(p_2)} = \frac{2\left(\sin(k_2)-\sin(k_1)\right)-iU}{2\left(\sin(k_2)-\sin(k_1)\right)+iU}.$$

For example, if $U=2+\sqrt{2}$ then two particles with momenta $k_1=-\pi/2$ and $k_2=\pi/4$ acquire a phase of $e^{-i\pi/2}=-i$ after scattering.

For a multi-particle quantum walk with nearest-neighbor interactions, $\mathcal{V}(|r|)=U\delta_{|r|,1}$ and $C=1$. In this case the eigenvalue equations for $|\psi(p_1;p_2)\rangle$ at $r=-1$, $r=1$, and $r=0$ are

$$\begin{aligned}
4\cos\left(\frac{p_1}{2}\right)\cos(p_2)(e^{ip_2}+R(p_1,p_2)e^{-ip_2}) &= U(e^{ip_2}+R(p_1,p_2)e^{-ip_2})\\
&\quad+2\cos\left(\frac{p_1}{2}\right)\left(e^{2ip_2}+R(p_1,p_2)e^{-2ip_2}+f(p_1,p_2,0)\right)\\
4\cos\left(\frac{p_1}{2}\right)\cos(p_2)T(p_1,p_2)e^{-ip_2} &= UT(p_1,p_2)e^{-ip_2}\\
&\quad+2\cos\left(\frac{p_1}{2}\right)\left(f(p_1,p_2,0)+T(p_1,p_2)e^{-2ip_2}\right)\\
2\cos(p_2)f(p_1,p_2,0) &= T(p_1,p_2)e^{-ip_2}+e^{ip_2}+R(p_1,p_2)e^{-ip_2},
\end{aligned}$$

respectively.

Solving these equations for R, T, and $f(p_1,p_2,0)$, we can construct the corresponding scattering states for bosons, fermions, or distinguishable particles (for more on the last case, see Section **??**). Unlike the case of the Bose-Hubbard model, we may not have $1+R=T$. For example, when $U=-2-\sqrt{2}$, $p_1=\pi/4$, and $p_2=3\pi/8$, we get $R=0$ and $T=i$ (see Section **??**).

5.1.2 Finite truncation

Theorem 2. *Let $H^{(2)}$ be a two-particle Hamiltonian of the form (5.1) with interaction range at most C, i.e., $\mathcal{V}(|r|)=0$ for all $|r|>C$. Let $\theta_\pm(p_1,p_2)$ be given by equation (5.6). Define $\theta=\theta_\pm(\pi/4,3\pi/8)$. Let $L\in\mathbb{N}^+$, let $M\in\{C+1,C+2,\ldots\}$, and define*

$$\begin{aligned}
|\chi_{z,k}\rangle &= \frac{1}{\sqrt{L}}\sum_{x=z-L}^{z-1} e^{ikx}|x\rangle\\
|\psi(0)\rangle &= \frac{1}{\sqrt{2}}\left(|\chi_{-M,-\frac{\pi}{2}}\rangle|\chi_{M+L+1,\frac{\pi}{4}}\rangle \pm |\chi_{M+L+1,\frac{\pi}{4}}\rangle|\chi_{-M,-\frac{\pi}{2}}\rangle\right).
\end{aligned}$$

Let c_0 be a constant independent of L. Then, for all $0\le t\le c_0L$, we have

$$\left\|e^{-iH^{(2)}t}|\psi(0)\rangle-|\alpha(t)\rangle\right\| = \emptyset(L^{-1/8}),$$

where

$$|\alpha(t)\rangle = \sum_{x,y} a_{xy}(t)|x,y\rangle, \tag{5.7}$$

$a_{xy}(t) = \pm a_{yx}(t)$, *and, for* $x \leq y$,

$$a_{xy}(t) = \frac{1}{\sqrt{2}L} e^{-\sqrt{2}it} \left[e^{-i\pi x/2} e^{i\pi y/4} F(x,y,t) \pm e^{i\theta} e^{i\pi x/4} e^{-i\pi y/2} F(y,x,t) \right] \tag{5.8}$$

where

$$F(u,v,t) = \begin{cases} 1 & \text{if } u - 2\lfloor t \rfloor \in \{-M-L,\ldots,-M-1\} \text{ and } v + 2\left\lfloor \frac{t}{\sqrt{2}} \right\rfloor \in \{M+1,\ldots,M+L\} \\ 0 & \text{otherwise.} \end{cases}$$

In this section we prove Theorem 2. The main proof appears in Section **??**, relying on several technical lemmas proved in Section 5.1.2.1. The proof follows the method used in the single-particle case, which is based on the calculation from the appendix of reference [**?**].

Recall from (5.5) that for each $p_1 \in (-\pi,\pi)$ and $p_2 \in (0,\pi)$ there is an eigenstate $|\mathrm{sc}(p_1;p_2)\rangle_\pm$ of $H^{(2)}$ of the form

$$\langle x,y|\mathrm{sc}(p_1;p_2)\rangle_\pm = \frac{e^{-ip_1\left(\frac{x+y}{2}\right)}}{\sqrt{2}} \begin{cases} e^{-ip_2(x-y)} \pm e^{i\theta_\pm(p_1,p_2)} e^{ip_2(x-y)} & \text{if } x-y \leq -C \\ e^{-ip_2(x-y)} e^{i\theta_\pm(p_1,p_2)} \pm e^{ip_2(x-y)} & \text{if } x-y \geq C \\ f(p_1,p_2,x-y) \pm f(p_1,p_2,y-x) & \text{if } |x-y| < C \end{cases} \tag{5.9}$$

where

$$e^{i\theta_\pm(p_1,p_2)} = T(p_1,p_2) \pm R(p_1,p_2),$$

C is the range of the interaction, T and R are the transmission and reflection coefficients of the interaction at the chosen momentum, f describes the amplitudes of the scattering state within the interaction range, and the $\pm$ depends on the type of particle ($+$ for bosons, $-$ for fermions). The state $|\mathrm{sc}(p_1;p_2)\rangle_\pm$ satisfies

$$H^{(2)}|\mathrm{sc}(p_1;p_2)\rangle_\pm = 4\cos\frac{p_1}{2}\cos p_2 |\mathrm{sc}(p_1;p_2)\rangle_\pm$$

and is delta-function normalized as

$$_\pm\langle \mathrm{sc}(p_1';p_2')|\mathrm{sc}(p_1;p_2)\rangle_\pm = 4\pi^2 \delta(p_1 - p_1')\delta(p_2 - p_2'). \tag{5.10}$$

Proof. Expand $|\psi(0)\rangle$ in the basis of eigenstates of the Hamiltonian to get

$$|\psi(t)\rangle = e^{-iH^{(2)}t}|\psi(0)\rangle = |\psi_1(t)\rangle + |\psi_2(t)\rangle$$

where

$$|\,\psi_1(t)\,\rangle = \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} e^{-it4\cos(\frac{p_1}{2}+\frac{\phi_1}{2})\cos(p_2+\phi_2)} |\mathrm{sc}(p_1+\phi_1;p_2+\phi_2)\rangle_\pm \left(_\pm\langle \mathrm{sc}(p_1+\phi_1;p_2+\phi_2)|\psi(0)\rangle\right)$$

with $D_\epsilon = [-\epsilon, \epsilon] \times [-\epsilon, \epsilon]$, $p_1 = \pi/2 - \pi/4 = \pi/4$, $p_2 = (\pi/2 + \pi/4)/2 = 3\pi/8$, and with $|\psi_2(t)\rangle$ orthogonal to $|\psi_1(t)\rangle$. We take $\epsilon = a/\sqrt{L}$ for some constant a. Using equation (5.9) we get

$$|\,\psi_1(t)\,\rangle = |\psi_A(t)\rangle \pm |\psi_B(t)\rangle$$

where

$$|\psi_A(t)\rangle = \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} e^{-it4\cos(\frac{\pi}{8}+\frac{\phi_1}{2})\cos(\frac{3\pi}{8}+\phi_2)} A(\phi_1,\phi_2) |\mathrm{sc}(\tfrac{\pi}{4}+\phi_1; \tfrac{3\pi}{8}+\phi_2)\rangle_\pm \tag{5.11}$$

$$|\,\psi_B(t)\,\rangle = \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} e^{-it4\cos(\frac{\pi}{8}+\frac{\phi_1}{2})\cos(\frac{3\pi}{8}+\phi_2)} e^{-i\theta_\pm(\frac{\pi}{4}+\phi_1, \frac{3\pi}{8}+\phi_2)} B(\phi_1,\phi_2,\tfrac{3\pi}{8}) |\mathrm{sc}(\tfrac{\pi}{4}+\phi_1; \tfrac{3\pi}{8}+\phi_2)\rangle_\pm$$

with

$$A(\phi_1,\phi_2) = \frac{1}{L} \sum_{x=-(M+L)}^{-(M+1)} \sum_{y=M+1}^{M+L} e^{i\phi_1 \frac{x+y}{2}} e^{i\phi_2(x-y)} \tag{5.12}$$

$$B(\phi_1,\phi_2,k) = \frac{1}{L} \sum_{x=-(M+L)}^{-(M+1)} \sum_{y=M+1}^{M+L} e^{i\phi_1 \frac{x+y}{2}} e^{i(\phi_2+2k)(y-x)}.$$

Using the delta-function normalization of the scattering states (equation (5.10)) we get

$$\begin{aligned}\langle\psi_B(t)|\psi_B(t)\rangle &= \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} \left|B(\phi_1,\phi_2,\tfrac{3\pi}{8})\right|^2 \\ &\leq \frac{16\pi^2}{L^2\epsilon^2}\end{aligned}$$

by Lemma 9 (as long as $\epsilon < 3\pi/8$, which holds for L sufficiently large). Similarly,

$$\begin{aligned}1 &\geq \langle\psi_A(t)|\psi_A(t)\rangle \\ &= \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} \left|A(\phi_1,\phi_2)\right|^2 \\ &\geq 1 - \frac{4\pi}{L\epsilon}\end{aligned}$$

(from the first two facts in Lemma 9) and therefore

$$\begin{aligned}\langle\psi_1(t)|\psi_1(t)\rangle &= \langle\psi_A(t)|\psi_A(t)\rangle + \langle\psi_B(t)|\psi_B(t)\rangle + \langle\psi_A(t)|\psi_B(t)\rangle + \langle\psi_B(t)|\psi_A(t)\rangle \\ &\geq 1 - \frac{4\pi}{L\epsilon} - 2\left|\langle\psi_A(t)|\psi_B(t)\rangle\right| \\ &\geq 1 - \frac{4\pi}{L\epsilon} - 2\left|\langle\psi_A(t)|\psi_A(t)\rangle\right|^{\frac{1}{2}} \left|\langle\psi_B(t)|\psi_B(t)\rangle\right|^{\frac{1}{2}} \\ &\geq 1 - \frac{12\pi}{L\epsilon}.\end{aligned}$$

Hence

$$\langle\psi_2(t)|\psi_2(t)\rangle \leq \frac{12\pi}{L\epsilon}$$

since

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi_1(t)|\psi_1(t)\rangle + \langle\psi_2(t)|\psi_2(t)\rangle = 1.$$

Thus

$$\begin{aligned}\| \, |\psi(t)\rangle - |\psi_A(t)\rangle\| &= \| \, |\psi_B(t)\rangle + |\psi_2(t)\rangle\| \\ &\leq \| \, |\psi_B(t)\rangle\| + \| \, |\psi_2(t)\rangle\| \\ &\leq \frac{4\pi}{L\epsilon} + \sqrt{\frac{12\pi}{L\epsilon}}.\end{aligned}$$

Now

$$\begin{aligned}\| \, |\psi(t)\rangle - |\alpha(t)\rangle\| &\leq \| \, |\psi(t)\rangle - |\psi_A(t)\rangle\| + \| \, |\psi_A(t)\rangle - |\alpha(t)\rangle\| \\ &\leq \frac{4\pi}{L\epsilon} + \sqrt{\frac{12\pi}{L\epsilon}} + \| \, |\psi_A(t)\rangle - |\alpha(t)\rangle\| \\ &= \emptyset(L^{-1/4}) + \| \, |\psi_A(t)\rangle - |\alpha(t)\rangle\|\end{aligned}$$

using our choice $\epsilon = a/\sqrt{L}$. To complete the proof, we now show that the second term in this expression is bounded by $\emptyset(L^{-1/8})$.

Lemma 7. *With $|\psi_A(t)\rangle$ and $|\alpha(t)\rangle$ defined through equations (5.11) and (5.7), with $t \leq c_0 L$ (for some constant c_0),*

$$\| \, |\psi_A(t)\rangle - |\alpha(t)\rangle\| = \emptyset(L^{-1/8}).$$

Proof. To simplify matters, note that both $|\psi_A(t)\rangle$ and $|\alpha(t)\rangle$ are either symmetric or anti-symmetric (i.e., $\langle x,y|\alpha(t)\rangle = \pm\langle y,x|\alpha(t)\rangle$ and $\langle x,y|\psi_A(t)\rangle = \pm\langle y,x|\psi_A(t)\rangle$). Taking C to be the maximum range of the interaction in our Hamiltonian, we have

$$\| \, |\psi_A(t)\rangle - |\alpha(t)\rangle\| \leq 2\left\|P_1|\psi_A(t)\rangle - P_1|\alpha(t)\rangle\right\| + \left\|P_2|\,\psi_A(t)\,\rangle\right\| + \left\|P_2|\,\alpha(t)\,\rangle\right\|,$$

where

$$P_1 = \sum_{y-x\geq C} |x,y\rangle\langle x,y| \qquad P_2 = \sum_{|x-y|<C} |\,x,y\,\rangle\langle\,x,y\,|.$$

Now, for $y - x \geq C$,

$$\begin{aligned}\langle x,y|\psi_A(t)\rangle &= \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} e^{-it4\cos(\frac{\pi}{8}+\frac{\phi_1}{2})\cos(\frac{3\pi}{8}+\phi_2)} A(\phi_1,\phi_2) \frac{e^{-i\left(\frac{\pi}{4}+\phi_1\right)\left(\frac{x+y}{2}\right)}}{\sqrt{2}} \\ &\quad \left(e^{i\left(\frac{3\pi}{8}+\phi_2\right)(y-x)} \pm e^{-i\left(\frac{3\pi}{8}+\phi_2\right)(y-x)+i\theta_\pm(\frac{\pi}{4}+\phi_1,\frac{3\pi}{8}+\phi_2)}\right) \\ &= \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} \left[\frac{1}{\sqrt{2}} e^{-it4\cos(\frac{\pi}{8}+\frac{\phi_1}{2})\cos(\frac{3\pi}{8}+\phi_2)} A(\phi_1,\phi_2)\right. \\ &\quad \left(e^{-i\pi x/2} e^{i\pi y/4} e^{-i\phi_1\left(\frac{x+y}{2}\right)} e^{i\phi_2(y-x)}\right. \\ &\quad \left.\left.\pm e^{i\pi x/4} e^{-i\pi y/2} e^{-i\phi_1\left(\frac{x+y}{2}\right)} e^{-i\phi_2(y-x)} e^{i\theta_\pm\left(\frac{\pi}{4}+\phi_1,\frac{3\pi}{8}+\phi_2\right)}\right)\right].\end{aligned}$$

From Lemma 10, for $x \le y$, the state $|\,\alpha(t)\,\rangle$ takes the form

$$\langle x,y|\alpha(t)\rangle = \frac{1}{\sqrt{2}}e^{-it\sqrt{2}}\Bigg[e^{-i\pi x/2}e^{i\pi y/4}\Bigg(\iint_{D_\pi}\frac{d\phi_1 d\phi_2}{4\pi^2} A(\phi_1,\phi_2)e^{-i\phi_1\left(-\lfloor t\rfloor+\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor+\frac{x+y}{2}\right)}e^{-2i\phi_2\left(-\lfloor t\rfloor-\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor+\frac{x-y}{2}\right)}\Bigg) \pm e^{i\theta}e^{i\pi x/4}e^{-i\pi y/2}\Bigg(\iint_{D_\pi}\frac{d\phi_1 d\phi_2}{4\pi^2} A(\phi_1,\phi_2)e^{-i\phi_1\left(-\lfloor t\rfloor+\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor+\frac{x+y}{2}\right)}e^{-2i\phi_2\left(-\lfloor t\rfloor-\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor+\frac{y-x}{2}\right)}\Bigg)\Bigg],$$

where $D_\pi = [-\pi,\pi]\times[-\pi,\pi]$. Using these expressions for $|\,\psi_A(t)\,\rangle$ and $|\,\alpha(t)\,\rangle$, we now write

$$P_1|\psi_A(t)\rangle - P_1|\alpha(t)\rangle = \pm|e_1(t)\rangle + |e_2(t)\rangle \pm |f_1(t)\rangle + |f_2(t)\rangle \pm |g_1(t)\rangle + |g_2(t)\rangle \pm |h(t)\rangle$$

where each term in the above equation is supported only on states $|x,y\rangle$ such that $y-x \ge C$, and (for $y-x\ge C$)

$$\langle x,y|e_1(t)\rangle = \frac{e^{i\theta}}{\sqrt{2}}e^{-it\sqrt{2}}e^{i\pi x/4}e^{-i\pi y/2}\iint_{D_\pi}\frac{d\phi_1 d\phi_2}{4\pi^2}A(\phi_1,\phi_2)\Bigg[e^{-i\phi_1\left(-t+\frac{t}{\sqrt{2}}+\frac{x+y}{2}\right)} e^{-2i\phi_2\left(-t-\frac{t}{\sqrt{2}}+\frac{y-x}{2}\right)} - e^{-i\phi_1\left(-\lfloor t\rfloor+\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor+\frac{x+y}{2}\right)}e^{-2i\phi_2\left(-\lfloor t\rfloor-\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor+\frac{y-x}{2}\right)}\Bigg]$$

$$\langle x,y|e_2(t)\rangle = \frac{1}{\sqrt{2}}e^{-it\sqrt{2}}e^{-i\pi x/2}e^{i\pi y/4}\iint_{D_\pi}\frac{d\phi_1 d\phi_2}{4\pi^2}A(\phi_1,\phi_2)\Bigg[e^{-i\phi_1\left(-t+\frac{t}{\sqrt{2}}+\frac{x+y}{2}\right)} e^{-2i\phi_2\left(-t-\frac{t}{\sqrt{2}}+\frac{x-y}{2}\right)} - e^{-i\phi_1\left(-\lfloor t\rfloor+\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor+\frac{x+y}{2}\right)}e^{-2i\phi_2\left(-\lfloor t\rfloor-\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor+\frac{x-y}{2}\right)}\Bigg]$$

$$\langle x,y|f_1(t)\rangle = -\frac{e^{i\theta}}{\sqrt{2}}e^{-it\sqrt{2}}e^{i\pi x/4}e^{-i\pi y/2}\iint_{D_\pi\setminus D_\epsilon}\frac{d\phi_1 d\phi_2}{4\pi^2}A(\phi_1,\phi_2) e^{-i\phi_1\left(-t+\frac{t}{\sqrt{2}}+\frac{x+y}{2}\right)}e^{-2i\phi_2\left(-t-\frac{t}{\sqrt{2}}+\frac{y-x}{2}\right)}$$

$$\langle x,y|f_2(t)\rangle = -\frac{1}{\sqrt{2}}e^{-it\sqrt{2}}e^{-i\pi x/2}e^{i\pi y/4}\iint_{D_\pi\setminus D_\epsilon}\frac{d\phi_1 d\phi_2}{4\pi^2}A(\phi_1,\phi_2) e^{-i\phi_1\left(-t+\frac{t}{\sqrt{2}}+\frac{x+y}{2}\right)}e^{-2i\phi_2\left(-t-\frac{t}{\sqrt{2}}+\frac{x-y}{2}\right)}$$

$$\langle x,y|g_1(t)\rangle = \frac{e^{i\theta}}{\sqrt{2}}e^{i\pi x/4}e^{-i\pi y/2}\iint_{D_\epsilon}\frac{d\phi_1 d\phi_2}{4\pi^2}A(\phi_1,\phi_2)e^{-i\phi_1\left(\frac{x+y}{2}\right)}e^{-2i\phi_2\left(\frac{y-x}{2}\right)} \left[e^{-it4\cos\left(\frac{\pi}{8}+\frac{\phi_1}{2}\right)\cos\left(\frac{3\pi}{8}+\phi_2\right)} - e^{-it\left(\sqrt{2}+\sqrt{2}\left(\frac{\phi_1}{2}-\phi_2\right)-2\left(\frac{\phi_1}{2}+\phi_2\right)\right)}\right]$$

$$\langle x,y|g_2(t)\rangle = \frac{1}{\sqrt{2}}e^{-i\pi x/2}e^{i\pi y/4}\iint_{D_\epsilon}\frac{d\phi_1 d\phi_2}{4\pi^2}A(\phi_1,\phi_2)e^{-i\phi_1\left(\frac{x+y}{2}\right)}e^{-2i\phi_2\left(\frac{x-y}{2}\right)} \left[e^{-it4\cos\left(\frac{\pi}{8}+\frac{\phi_1}{2}\right)\cos\left(\frac{3\pi}{8}+\phi_2\right)} - e^{-it\left(\sqrt{2}+\sqrt{2}\left(\frac{\phi_1}{2}-\phi_2\right)-2\left(\frac{\phi_1}{2}+\phi_2\right)\right)}\right]$$

$$\langle x,y|h(t)\rangle = \frac{1}{\sqrt{2}}e^{i\pi x/4}e^{-i\pi y/2}\iint_{D_\epsilon}\frac{d\phi_1 d\phi_2}{4\pi^2}A(\phi_1,\phi_2)e^{-i\phi_1\left(\frac{x+y}{2}\right)}e^{-2i\phi_2\left(\frac{y-x}{2}\right)} e^{-it4\cos\left(\frac{\pi}{8}+\frac{\phi_1}{2}\right)\cos\left(\frac{3\pi}{8}+\phi_2\right)}\left(e^{i\theta_\pm\left(\frac{\pi}{4}+\phi_1,\frac{3\pi}{8}+\phi_2\right)} - e^{i\theta}\right).$$

We now proceed to bound the norm of each of these states. We repeatedly use the fact that, for $(\phi_1, \phi_2) \in D_\pi$,

$$\sum_{x,y=-\infty}^{\infty} e^{ix\left(\frac{1}{2}(\phi_1-\tilde{\phi}_1)-(\phi_2-\tilde{\phi}_2)\right)} e^{iy\left(\frac{1}{2}(\phi_1-\tilde{\phi}_1)+(\phi_2-\tilde{\phi}_2)\right)} = 4\pi^2 \delta(\phi_1 - \tilde{\phi}_1)\delta(\phi_2 - \tilde{\phi}_2).$$

Using this formula we get

$$\begin{aligned}
\langle e_1(t)|e_1(t)\rangle &= \sum_{y-x\geq C} \langle e_1(t)|x,y\rangle\langle x,y|e_1(t)\rangle \\
&\leq \sum_{x=-\infty}^{\infty}\sum_{y=-\infty}^{\infty} \Bigg| \frac{1}{\sqrt{2}} \iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2} A(\phi_1,\phi_2) \Big[e^{-i\phi_1\left(-t+\frac{t}{\sqrt{2}}+\frac{x+y}{2}\right)} \\
&\qquad e^{-2i\phi_2\left(-t-\frac{t}{\sqrt{2}}+\frac{y-x}{2}\right)} - e^{-i\phi_1\left(-\lfloor t\rfloor+\left\lfloor \frac{t}{\sqrt{2}}\right\rfloor+\frac{x+y}{2}\right)} e^{-2i\phi_2\left(-\lfloor t\rfloor-\left\lfloor \frac{t}{\sqrt{2}}\right\rfloor+\frac{y-x}{2}\right)} \Big] \Bigg|^2 \\
&= \frac{1}{2} \iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2} |A(\phi_1,\phi_2)|^2 \Big| e^{-i\phi_1\left(-t+\frac{t}{\sqrt{2}}\right)} e^{-2i\phi_2\left(-t-\frac{t}{\sqrt{2}}\right)} \\
&\qquad - e^{-i\phi_1\left(-\lfloor t\rfloor+\left\lfloor \frac{t}{\sqrt{2}}\right\rfloor\right)} e^{-2i\phi_2\left(-\lfloor t\rfloor-\left\lfloor \frac{t}{\sqrt{2}}\right\rfloor\right)} \Big|^2 .
\end{aligned}$$

Now use the fact that $|e^{-ic} - 1|^2 \leq c^2$ for $c \in \mathbb{R}$ to get

$$\begin{aligned}
\langle e_1(t)|e_1(t)\rangle &\leq \frac{1}{2} \iint_{D_\pi} \left(\frac{d\phi_1 d\phi_2}{4\pi^2}\right) |A(\phi_1,\phi_2)|^2 \Bigg(-\phi_1 \left(-t + \frac{t}{\sqrt{2}} + \lfloor t\rfloor - \left\lfloor \frac{t}{\sqrt{2}}\right\rfloor\right) \\
&\qquad - 2\phi_2 \left(-t - \frac{t}{\sqrt{2}} + \lfloor t\rfloor + \left\lfloor \frac{t}{\sqrt{2}}\right\rfloor\right)\Bigg)^2 \\
&\leq 4 \iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2} |A(\phi_1,\phi_2)|^2 \left(\phi_1^2 + 4\phi_2^2\right)
\end{aligned}$$

using the Cauchy-Schwarz inequality and the fact that $\left|t - t/\sqrt{2} - \lfloor t\rfloor - \lfloor t/\sqrt{2}\rfloor\right| \leq 2$. So

$$\begin{aligned}
\langle e_1(t)|e_1(t)\rangle &\leq 4 \left(\iint_{D_\pi \setminus D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} + \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} \right) |A(\phi_1,\phi_2)|^2 \left(\phi_1^2 + 4\phi_2^2\right) \\
&\leq 4\left(5\pi^2\right)\left(\frac{4\pi}{L\epsilon}\right) + 20\epsilon^2 \\
&= \frac{80\pi^3}{L\epsilon} + 20\epsilon^2
\end{aligned}$$

where we have used Lemma 9 and the fact that $\phi_1^2 + 4\phi_2^2 \leq 5\epsilon^2$ on D_ϵ. Similarly,

$$\langle e_2(t)|e_2(t)\rangle \leq \frac{80\pi^3}{L\epsilon} + 20\epsilon^2.$$

Now

$$\begin{aligned}\langle f_1(t)|f_1(t)\rangle &\leq \frac{1}{2}\iint_{D_\pi\setminus D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2}\,|A(\phi_1,\phi_2)|^2 \\ &\leq \frac{2\pi}{L\epsilon}\end{aligned}$$

by Lemma 9, and similarly

$$\langle f_2(t)|f_2(t)\rangle \leq \frac{2\pi}{L\epsilon}.$$

Moving on to the next term,

$$\begin{aligned}\langle g_1(t)|g_1(t)\rangle &\leq \frac{1}{2}\iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2}\,|A(\phi_1,\phi_2)|^2 \Big| e^{-it4\cos\left(\frac{\pi}{8}+\frac{\phi_1}{2}\right)\cos\left(\frac{3\pi}{8}+\phi_2\right)} \\ &\qquad - e^{-it\left(\sqrt{2}+\sqrt{2}\left(\frac{\phi_1}{2}-\phi_2\right)-2\left(\frac{\phi_1}{2}+\phi_2\right)\right)}\Big|^2 \\ &\leq \frac{1}{2}\iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2}\Bigg[|A(\phi_1,\phi_2)|^2\, t^2\left(4\cos\left(\frac{\pi}{8}+\frac{\phi_1}{2}\right)\cos\left(\frac{3\pi}{8}+\phi_2\right)\right. \\ &\qquad \left. -\sqrt{2}-\sqrt{2}\left(\frac{\phi_1}{2}-\phi_2\right)+2\left(\frac{\phi_1}{2}+\phi_2\right)\right)^2\Bigg] \end{aligned} \tag{5.13}$$

using $|e^{-ic}-1|^2 \leq c^2$ for $c \in \mathbb{R}$. Now

$$\begin{aligned}4\cos\left(\frac{\pi}{8}+\frac{\phi_1}{2}\right)\cos\left(\frac{3\pi}{8}+\phi_2\right) &= 2\cos\left(\frac{\pi}{2}+\frac{\phi_1}{2}+\phi_2\right)+2\cos\left(-\frac{\pi}{4}+\frac{\phi_1}{2}-\phi_2\right) \\ &= -2\sin\left(\frac{\phi_1}{2}+\phi_2\right)+\sqrt{2}\cos\left(\frac{\phi_1}{2}-\phi_2\right)+\sqrt{2}\sin\left(\frac{\phi_1}{2}-\phi_2\right)\end{aligned}$$

so

$$\begin{aligned}&\left|4\cos\left(\frac{\pi}{8}+\frac{\phi_1}{2}\right)\cos\left(\frac{3\pi}{8}+\phi_2\right)-\sqrt{2}-\sqrt{2}\left(\frac{\phi_1}{2}-\phi_2\right)+2\left(\frac{\phi_1}{2}+\phi_2\right)\right| \\ &\quad \leq \left|\sqrt{2}\left(\cos\left(\frac{\phi_1}{2}-\phi_2\right)-1\right)\right| + \left|\sqrt{2}\left(\sin\left(\frac{\phi_1}{2}-\phi_2\right)-\left(\frac{\phi_1}{2}-\phi_2\right)\right)\right| \\ &\qquad + \left|2\left(\sin\left(\frac{\phi_1}{2}+\phi_2\right)-\left(\frac{\phi_1}{2}+\phi_2\right)\right)\right| \\ &\quad \leq \sqrt{2}\left(\frac{\phi_1}{2}-\phi_2\right)^2+\sqrt{2}\left(\frac{\phi_1}{2}-\phi_2\right)^2+2\left(\frac{\phi_1}{2}+\phi_2\right)^2 \\ &\quad \leq 4\left(\left(\frac{\phi_1}{2}+\phi_2\right)^2+\left(\frac{\phi_1}{2}-\phi_2\right)^2\right),\end{aligned}$$

using $|\cos x - 1| \leq x^2$ and $|\sin x - x| \leq x^2$ for $x \in \mathbb{R}$. Plugging this into equation (5.13) we get

$$\begin{aligned}
\langle g_1(t)|g_1(t)\rangle &\leq \frac{1}{2}\iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} 16\,|A(\phi_1,\phi_2)|^2\, t^2 \left(\left(\frac{\phi_1}{2}+\phi_2\right)^2 + \left(\frac{\phi_1}{2}-\phi_2\right)^2\right)^2 \\
&\leq 16t^2 \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} |A(\phi_1,\phi_2)|^2 \left(\left(\frac{\phi_1}{2}+\phi_2\right)^4 + \left(\frac{\phi_1}{2}-\phi_2\right)^4\right) \\
&\leq \frac{16t^2}{L^2} \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} \frac{\sin^2(\frac{L}{2}[\frac{\phi_1}{2}+\phi_2])}{\sin^2(\frac{1}{2}[\frac{\phi_1}{2}+\phi_2])} \frac{\sin^2(\frac{L}{2}[-\frac{\phi_1}{2}+\phi_2])}{\sin^2(\frac{1}{2}[-\frac{\phi_1}{2}+\phi_2])} \\
&\qquad \left(\left(\frac{\phi_1}{2}+\phi_2\right)^4 + \left(\frac{\phi_1}{2}-\phi_2\right)^4\right)
\end{aligned}$$

where we used the Cauchy-Schwarz inequality in the second line and equation (5.17) in the last line. Changing coordinates to

$$\alpha_1 = \phi_1 + \frac{\phi_2}{2} \qquad \alpha_2 = \frac{\phi_1}{2} - \phi_2$$

and realizing that $|\alpha_1|, |\alpha_2| < 3\epsilon/2$ for $(\phi_1,\phi_2) \in D_\epsilon$, we see that

$$\begin{aligned}
\langle g_1(t)\,|g_1(t)\rangle &\leq \frac{16t^2}{L^2}\int_{-3\epsilon/2}^{3\epsilon/2} \frac{d\alpha_1}{2\pi} \int_{-3\epsilon/2}^{3\epsilon/2} \frac{d\alpha_1}{2\pi} \frac{\sin^2(\frac{1}{2}L\alpha_1)}{\sin^2(\frac{1}{2}\alpha_1)} \frac{\sin^2(\frac{1}{2}L\alpha_2)}{\sin^2(\frac{1}{2}\alpha_2)} \left(\alpha_1^4 + \alpha_2^4\right) \\
&= \frac{32t^2}{L^2}\int_{-3\epsilon/2}^{3\epsilon/2} \frac{d\alpha_1}{2\pi} \int_{-3\epsilon/2}^{3\epsilon/2} \frac{d\alpha_1}{2\pi} \frac{\sin^2(\frac{1}{2}L\alpha_1)}{\sin^2(\frac{1}{2}\alpha_1)} \frac{\sin^2(\frac{1}{2}L\alpha_2)}{\sin^2(\frac{1}{2}\alpha_2)} \alpha_1^4 \\
&\leq \frac{32t^2}{L}\int_{-3\epsilon/2}^{3\epsilon/2} \frac{d\alpha_1}{2\pi} \frac{\sin^2(\frac{1}{2}L\alpha_1)}{\sin^2(\frac{1}{2}\alpha_1)} \alpha_1^4 \\
&\leq \frac{32t^2}{L}\int_{-3\epsilon/2}^{3\epsilon/2} \frac{d\alpha_1}{2\pi} \frac{\pi^2}{\alpha_1^2} \alpha_1^4 \\
&= \frac{36\pi t^2 \epsilon^3}{L},
\end{aligned}$$

with a similar bound on $\langle g_2(t)|g_2(t)\rangle$.

Finally,

$$\langle h(t)|h(t)\rangle \leq \frac{1}{2}\iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} |A(\phi_1,\phi_2)|^2 \left| e^{i\theta_\pm(\frac{\pi}{4}+\phi_1, \frac{3\pi}{8}+\phi_2)} - e^{i\theta}\right|^2.$$

Recall that $e^{i\theta_\pm(p_1,p_2)} = T(p_1,p_2) \pm R(p_1,p_2)$ is obtained by solving for the effective single-particle S-matrix for the Hamiltonian (5.3). For p_1 near $\pi/4$ we divide this Hamiltonian by $2\cos(p_1/2)$ to put it in the form considered in [**?**], where the potential term is now $\mathcal{V}(|r|)/(2\cos(p_1/2))$. The entries $T(p_1,p_2)$ and $R(p_1,p_2)$ of this S-matrix are bounded rational functions of $z = e^{ip_2}$ and $(2\cos(p_1/2))^{-1}$ [**?**], so they are differentiable as a function of p_1 and

p_2 on some neighborhood U of $(\pi/4, 3\pi/8)$ (and have bounded partial derivatives on this neighborhood).

For ϵ small enough that $D_\epsilon \subset U$ we get, using the mean value theorem and the fact that $\theta = \theta_\pm(\pi/4, 3\pi/8)$,

$$\begin{aligned}\left| e^{i\theta_\pm(\frac{\pi}{4}+\phi_1, \frac{3\pi}{8}+\phi_2)} - e^{i\theta} \right| &\le \sqrt{\phi_1^2+\phi_2^2} \max_U \left| \vec{\nabla} e^{i\theta_\pm} \right| \quad \text{for } (\phi_1,\phi_2) \in D_\epsilon \\ &\le \epsilon\Gamma\end{aligned}$$

for some constant Γ (independent of L). Therefore

$$\begin{aligned}\langle h(t)|h(t)\rangle &\le \frac{1}{2} \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} \left|A(\phi_1,\phi_2)\right|^2 \epsilon^2\Gamma^2 \\ &\le \frac{1}{2}\Gamma^2\epsilon^2.\end{aligned}$$

Putting these bounds together, we get

$$\begin{aligned}\|P_1|\psi_A(t)\rangle - P_1|\alpha(t)\rangle\| &\le \||e_1(t)\rangle\| + \||e_2(t)\rangle\| + \||f_1(t)\rangle\| + \||f_2(t)\rangle\| \\ &\quad + \||g_1(t)\rangle\| + \||g_2(t)\rangle\| + \||h(t)\rangle\| \\ &\le 2\left(\frac{80\pi^3}{L\epsilon} + 20\epsilon^2\right)^{\frac{1}{2}} + 2\left(\frac{2\pi}{L\epsilon}\right)^{\frac{1}{2}} + 2\left(\frac{36\pi t^2\epsilon^3}{L}\right)^{\frac{1}{2}} + \frac{1}{\sqrt{2}}\Gamma\epsilon.\end{aligned}$$

Letting $\epsilon = a/\sqrt{L}$ and $t \le c_0 L$ we get

$$\| P_1|\psi_A(t)\rangle - P_1|\alpha(t)\rangle\| = \emptyset(L^{-1/4}). \tag{5.14}$$

Since $P_2|\,\alpha(t)\,\rangle$ has support on at most $4CL$ basis states $|x,y\rangle$, and since $|\langle x,y|P_2|\alpha(t)\rangle|^2 = \emptyset(L^{-2})$, we get

$$\|P_2|\,\alpha(t)\,\rangle\| = \emptyset(L^{-1/2}). \tag{5.15}$$

We now use the bounds (5.14) and (5.15) and Lemma 8 to show that

$$\||\psi_A(t)\rangle - |\alpha(t)\rangle\| = \emptyset(L^{-1/8}). \tag{5.16}$$

First consider the case where the interaction range is $C = 0$ (as in the Bose-Hubbard model). In this case equation (5.16) follows directly from equation (5.14) and the facts that $\langle x,y|\alpha(t)\rangle = \pm\langle y,x|\alpha(t)\rangle$ and $\langle x,y|\psi_A(t)\rangle = \pm\langle y,x|\psi_A(t)\rangle$.

Now suppose $C \ne 0$. In this case

$$\begin{aligned}\|(1-P_2)\,|\psi_A(t)\rangle\|^2 &= 2\,\|P_1|\psi_A(t)\rangle\|^2 \\ &= 2\left(\|P_1|\alpha(t)\rangle\| + \emptyset(L^{-1/4})\right)^2 \\ &= 2\left(\frac{1}{2}\,\|(1-P_2)|\alpha(t)\rangle\|^2 + \emptyset(L^{-1/4})\right) \\ &= 1 + \emptyset(L^{-1}) - \langle\alpha(t)|P_2|\alpha(t)\rangle + \emptyset(L^{-1/4}) \\ &= 1 + \emptyset(L^{-1/4})\end{aligned}$$

where in the next-to-last line we have used Lemma 8. So

$$\begin{aligned}\||\psi_A(t)\rangle - |\alpha(t)\rangle\| &\leq 2\left\|P_1|\psi_A(t)\rangle - P_1|\alpha(t)\rangle\right\| + \|P_2|\alpha(t)\rangle\| + \|P_2|\psi_A(t)\rangle\| \\ &= \emptyset(L^{-1/4}) + \emptyset(L^{-1/2}) + (1 - \|(1-P_2)\,|\psi_A(t)\rangle\|)^{\frac{1}{2}} \\ &= \emptyset(L^{-1/4}) + \emptyset(L^{-1/2}) + \emptyset(L^{-1/8}) \\ &= \emptyset(L^{-1/8})\end{aligned}$$

which completes the proof. □

□

5.1.2.1 Technical lemmas

In this section we prove three lemmas that are used in the proof of Theorem 2.

Lemma 8. *Let $|\alpha(t)\rangle$ be defined as in Theorem 2. Then*

$$\langle\alpha(t)|\alpha(t)\rangle = 1 + \emptyset(L^{-1}).$$

Proof. Define

$$\Pi = \sum_{x\leq y} |x,y\rangle\langle x,y|.$$

Note that, since $\langle x,y|\alpha(t)\rangle = \pm\langle y,x|\alpha(t)\rangle$,

$$\begin{aligned}\langle\alpha(t)|\alpha(t)\rangle &= 2\langle\alpha(t)|\Pi|\alpha(t)\rangle - \sum_{x=-\infty}^{\infty}\langle\alpha(t)|x,x\rangle\langle x,x|\alpha(t)\rangle \\ &= 2\langle\alpha(t)|\Pi|\alpha(t)\rangle + \emptyset(L^{-1})\end{aligned}$$

where the last line follows since $|\langle x,x|\alpha(t)\rangle|^2$ is nonzero for at most L values of x and $|\langle x,x|\alpha(t)\rangle|^2 = \emptyset(L^{-2})$. We now show that

$$\langle\alpha(t)|\Pi|\alpha(t)\rangle = \frac{1}{2} + O(L^{-1}).$$

Note that

$$\begin{aligned}\langle\alpha(t)|\Pi|\alpha(t)\rangle = \frac{1}{2L^2}\sum_{x\leq y}\Bigg(&F(x,y,t) + F(y,x,t) \\ &\pm e^{i\theta}e^{\frac{3i\pi}{4}x}e^{-\frac{3i\pi}{4}y}F(x,y,t)F(y,x,t) \\ &\pm e^{-i\theta}e^{-\frac{3i\pi}{4}x}e^{\frac{3i\pi}{4}y}F(x,y,t)F(y,x,t)\Bigg).\end{aligned}$$

Now $F(x,y,t) = 1$ if and only if $x \in \{-M-L+2\lfloor t\rfloor,\ldots,-M-1+2\lfloor t\rfloor\}$ and $y \in \{M+1-2\lfloor t/\sqrt{2}\rfloor,\ldots,M+L-2\lfloor t/\sqrt{2}\rfloor\}$. Similarly $F(y,x,t) = 1$ if and only if $x \in \{M+1-2\lfloor t/\sqrt{2}\rfloor,\ldots,M+L-2\lfloor t/\sqrt{2}\rfloor\}$ and $y \in \{-M-L+2\lfloor t\rfloor,\ldots,-M-1+2\lfloor t\rfloor\}$. So

$$\sum_{x\leq y} F(y,x,t) = \sum_{y\leq x} F(x,y,t)$$

and

$$\frac{1}{2L^2}\sum_{x\le y}\left[F(x,y,t)+F(y,x,t)\right]=\frac{1}{2L^2}\left(\sum_{x=-\infty}^{\infty}\sum_{y=-\infty}^{\infty}F(x,y,t)-\sum_{x=-\infty}^{\infty}F(x,x,t)\right)$$
$$=\frac{1}{2}+\emptyset(L^{-1}).$$

We now establish the bound

$$\left|\frac{1}{2L^2}\sum_{x\le y}e^{\frac{3i\pi}{4}x}e^{-\frac{3i\pi}{4}y}F(x,y,t)F(y,x,t)\right|=\emptyset(L^{-1})$$

to complete the proof. To get this bound, note that both $F(x,y,t)=1$ and $F(y,x,t)=1$ if and only if

$$x,y\in\{-M-L+2\lfloor t\rfloor,\dots,-M-1+2\lfloor t\rfloor\}$$
$$\text{and } x,y\in\left\{M+1-2\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor,\dots,M+L-2\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor\right\}.$$

Letting

$$B=\{-M-L+2\lfloor t\rfloor,\dots,-M-1+2\lfloor t\rfloor\}\cap\left\{M+1-2\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor,\dots,M+L-2\left\lfloor\frac{t}{\sqrt{2}}\right\rfloor\right\},$$

we have

$$B=\{j,j+1,\dots,j+l\}$$

for some $j,l\in\mathbb{Z}$ with $l<L$. So

$$\frac{1}{2L^2}\left|\sum_{x\le y}e^{\frac{3i\pi}{4}x}e^{-\frac{3i\pi}{4}y}F(x,y,t)F(y,x,t)\right|=\frac{1}{2L^2}\left|\sum_{x,y\in B,\,x\le y}e^{\frac{3i\pi}{4}x}e^{-\frac{3i\pi}{4}y}\right|$$
$$=\frac{1}{2L^2}\left|\sum_{y=j}^{j+l}\sum_{x=j}^{y}e^{\frac{3i\pi}{4}x}e^{-\frac{3i\pi}{4}y}\right|$$
$$=\frac{1}{2L^2}\left|\sum_{y=j}^{j+l}e^{-\frac{3i\pi}{4}y}e^{3i\frac{\pi}{4}j}\frac{e^{3i\frac{\pi}{4}(y+1-j)}-1}{e^{3i\frac{\pi}{4}}-1}\right|$$
$$\le\frac{(l+1)}{2L^2}\frac{2}{\left|e^{3i\frac{\pi}{4}}-1\right|}$$
$$=\emptyset(L^{-1})$$

since $l<L$. □

Lemma 9. *Let $k\in(-\pi,0)\cup(0,\pi)$ and $0<\epsilon<\min\{\pi-|k|,|k|\}$. Let*

$$D_\epsilon=[-\epsilon,\epsilon]\times[-\epsilon,\epsilon]$$
$$D_\pi=[-\pi,\pi]\times[-\pi,\pi].$$

Then

$$\iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2}|A(\phi_1,\phi_2)|^2 = 1$$
$$\iint_{D_\pi\setminus D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2}|A(\phi_1,\phi_2)|^2 \le \frac{4\pi}{L\epsilon}$$
$$\iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2}|B(\phi_1,\phi_2,k)|^2 \le \frac{4\pi^2}{L^2\epsilon^2}.$$

where $A(\phi_1,\phi_2)$ *and* $B(\phi_1,\phi_2,k)$ *are given by equation (5.12).*

Proof. Using equation (5.12) we get

$$|A(\phi_1,\phi_2)|^2 = \frac{1}{L^2}\sum_{x,\tilde{x}=-(M+L)}^{-(M+1)}\sum_{y,\tilde{y}=M+1}^{M+L} e^{i\frac{\phi_1}{2}(x+y-(\tilde{x}+\tilde{y}))}e^{i\phi_2(x-y-(\tilde{x}-\tilde{y}))}.$$

Now

$$\int_{-\pi}^{\pi}\frac{d\phi_2}{2\pi}e^{i\phi_2(x-y-\tilde{x}+\tilde{y})} = \delta_{x-y,\tilde{x}-\tilde{y}},$$

so (suppressing the limits of summation for readability)

$$\begin{aligned}\iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2}|A(\phi_1,\phi_2)|^2 &= \frac{1}{L^2}\int_{-\pi}^{\pi}\frac{d\phi_1}{2\pi}\sum_{x,\tilde{x}}\sum_{y,\tilde{y}} e^{i\phi_1(y-\tilde{y})}\delta_{x-y,\tilde{x}-\tilde{y}}\\ &= \frac{1}{L^2}\sum_{x,\tilde{x}}\sum_{y,\tilde{y}}\delta_{y,\tilde{y}}\delta_{x-y,\tilde{x}-\tilde{y}}\\ &= 1\end{aligned}$$

which proves the first part.

By performing the sums in equation (5.12) we get

$$|A(\phi_1,\phi_2)|^2 = \frac{1}{L^2}\frac{\sin^2(\frac{1}{2}L[\frac{\phi_1}{2}+\phi_2])}{\sin^2(\frac{1}{2}[\frac{\phi_1}{2}+\phi_2])}\frac{\sin^2(\frac{1}{2}L[\frac{\phi_1}{2}-\phi_2])}{\sin^2(\frac{1}{2}[\frac{\phi_1}{2}-\phi_2])}. \tag{5.17}$$

Letting $\alpha_1 = \phi_1/2+\phi_2$ and $\alpha_2 = \phi_1/2-\phi_2$, we see that $|\alpha_1| \le 3\pi/2$, $|\alpha_2| \le 3\pi/2$, and $\alpha_1^2+\alpha_2^2 \ge 5\epsilon^2/2$ whenever $(\phi_1,\phi_2) \in D_\pi \setminus D_\epsilon$. Defining $D_{3\pi/2} = [-3\pi/2, 3\pi/2]^2$ we get

$(\alpha_1, \alpha_2) \in D_{3\pi/2} \setminus D_\epsilon$ whenever $(\phi_1, \phi_2) \in D_\pi \setminus D_\epsilon$. Hence

$$\begin{aligned}
\iint_{D_\pi \setminus D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} |A(\phi_1, \phi_2)|^2 &\leq \frac{1}{L^2} \iint_{D_{3\pi/2} \setminus D_\epsilon} \frac{d\alpha_1 d\alpha_2}{4\pi^2} \frac{\sin^2(\frac{1}{2}L\alpha_1)}{\sin^2(\frac{1}{2}\alpha_1)} \frac{\sin^2(\frac{1}{2}L\alpha_2)}{\sin^2(\frac{1}{2}\alpha_2)} \\
&\leq \frac{4}{L} \left(\frac{1}{L} \int_{-\frac{3\pi}{2}}^{\frac{3\pi}{2}} \frac{d\alpha_1}{2\pi} \frac{\sin^2(\frac{1}{2}L\alpha_1)}{\sin^2(\frac{1}{2}\alpha_1)} \right) \left(\int_\epsilon^{3\pi/2} \frac{d\alpha_2}{2\pi} \frac{\sin^2(\frac{1}{2}L\alpha_2)}{\sin^2(\frac{1}{2}\alpha_2)} \right) \\
&\leq \frac{4}{L} \left(\int_{-2\pi}^{2\pi} \frac{d\alpha_1}{2\pi} \frac{1}{L} \frac{\sin^2(\frac{1}{2}L\alpha_1)}{\sin^2(\frac{1}{2}\alpha_1)} \right) \left(\int_\epsilon^{\frac{3\pi}{2}} \frac{d\alpha_2}{2\pi} \frac{1}{\sin^2(\frac{1}{2}\alpha_2)} \right) \\
&= \frac{8}{L} \left(\int_\epsilon^\pi \frac{d\alpha_2}{2\pi} \frac{1}{\sin^2(\frac{1}{2}\alpha_2)} + \int_\pi^{\frac{3\pi}{2}} \frac{d\alpha_2}{2\pi} \frac{1}{\sin^2(\frac{1}{2}\alpha_2)} \right) \\
&\leq \frac{8}{L} \left(\int_\epsilon^\pi \frac{d\alpha_2}{2\pi} \frac{\pi^2}{\alpha_2^2} + 2 \int_\pi^{\frac{3\pi}{2}} \frac{d\alpha_2}{2\pi} \right) \\
&= \frac{4\pi}{L\epsilon}
\end{aligned}$$

which proves the second inequality (in the next-to-last line we have used the fact that $\sin(x/2) > x/\pi$ for $x \in (0, \pi)$ and $\sin^2(x/2) > 1/2$ for $x \in (\pi, 3\pi/2)$).

Now

$$\begin{aligned}
|B(\phi_1, \phi_2, k)|^2 &= |A(\phi_1, -\phi_2 - 2k)|^2 \\
&\leq \frac{1}{L^2} \frac{1}{\sin^2\left(\frac{1}{2}\left[\frac{\phi_1}{2} + \phi_2 + 2k\right]\right)} \frac{1}{\sin^2\left(\frac{1}{2}\left[-\frac{\phi_1}{2} + \phi_2 + 2k\right]\right)}.
\end{aligned}$$

If $(\phi_1, \phi_2) \in D_\epsilon$ then $|k| - 3\epsilon/4 \leq |\pm\phi_1/4 + \phi_2/2 + k| \leq |k| + 3\epsilon/4$. Noting that ϵ is chosen such that $0 < \epsilon < \min\{\pi - |k|, |k|\}$, we get

$$\frac{\epsilon}{4} \leq \left| \pm\frac{\phi_1}{4} + \frac{\phi_2}{2} + k \right| \leq \pi - \frac{\epsilon}{4}$$

so

$$\begin{aligned}
|B(\phi_1, \phi_2, k)|^2 &\leq \frac{1}{L^2} \frac{1}{\sin^4(\frac{\epsilon}{4})} \\
&\leq \frac{16\pi^4}{L^2\epsilon^4}
\end{aligned}$$

and

$$\begin{aligned}
\iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} |B(\phi_1, \phi_2, k)|^2 &\leq \frac{1}{4\pi^2} (2\epsilon)^2 \left(\frac{16\pi^4}{L^2\epsilon^4} \right) \\
&= \frac{16\pi^2}{L^2\epsilon^2}.
\end{aligned}$$

□

Lemma 10. *Let $a_{xy}(t)$ be as in Theorem 2. For $x \leq y$,*

$$a_{xy}(t) = \frac{1}{\sqrt{2}} e^{-it\sqrt{2}} \Bigg[e^{-i\pi x/2} e^{i\pi y/4} \Bigg(\iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2} A(\phi_1, \phi_2) \\ e^{-i\phi_1 \left(-\lfloor t \rfloor + \lfloor \frac{t}{\sqrt{2}} \rfloor + \frac{x+y}{2}\right)} e^{-2i\phi_2 \left(-\lfloor t \rfloor - \lfloor \frac{t}{\sqrt{2}} \rfloor + \frac{x-y}{2}\right)} \Bigg) \\ \pm e^{i\theta} e^{i\pi x/4} e^{-i\pi y/2} \Bigg(\iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2} A(\phi_1, \phi_2) \\ e^{-i\phi_1 \left(-\lfloor t \rfloor + \lfloor \frac{t}{\sqrt{2}} \rfloor + \frac{x+y}{2}\right)} e^{-2i\phi_2 \left(-\lfloor t \rfloor - \lfloor \frac{t}{\sqrt{2}} \rfloor + \frac{y-x}{2}\right)} \Bigg) \Bigg].$$

Proof. The lemma follows from (5.8) and the fact that, for any two numbers γ_1, γ_2 such that $\gamma_1 + \gamma_2, \gamma_1 - \gamma_2 \in \mathbb{Z}$,

$$\iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2} A(\phi_1, \phi_2) e^{i\gamma_1 \phi_1 + 2i\gamma_2 \phi_2} = \begin{cases} \frac{1}{L} & \text{if } (-\gamma_1 - \gamma_2, -\gamma_1 + \gamma_2) \in S \\ 0 & \text{otherwise} \end{cases}$$

where $S = \{-M-L, \ldots, -M-1\} \times \{M+1, \ldots, M+L\}$. To establish this formula, observe that

$$\begin{aligned} \iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2} A(\phi_1, \phi_2) e^{i\gamma_1 \phi_1 + 2i\gamma_2 \phi_2} &= \frac{1}{L} \sum_{x=-M-L}^{-M-1} \sum_{y=M+1}^{M+L} \iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2} e^{i\phi_1 \left(\gamma_1 + \frac{x+y}{2}\right)} e^{i\phi_2 (x-y+2\gamma_2)} \\ &= \frac{1}{L} \sum_{x=-M-L}^{-M-1} \sum_{y=M+1}^{M+L} \int_{-\pi}^{\pi} \frac{d\phi_1}{2\pi} e^{i\phi_1 \left(\gamma_1 + \frac{x-y}{2}\right)} \delta_{y,-x-2\gamma_2}. \end{aligned}$$

Here we have performed the integral over ϕ_2 using the fact that $2\gamma_2$ is an integer. We then have

$$\begin{aligned} \iint_{D_\pi} \frac{d\phi_1 d\phi_2}{4\pi^2} A(\phi_1, \phi_2) e^{i\gamma_1 \phi_1 + 2i\gamma_2 \phi_2} &= \frac{1}{L} \sum_{x=-M-L}^{-M-1} \sum_{y=M+1}^{M+L} \int_{-\pi}^{\pi} \frac{d\phi_1}{2\pi} e^{i\phi_1 (\gamma_1 + x + \gamma_2)} \delta_{y,-x-2\gamma_1} \\ &= \frac{1}{L} \sum_{x=-M-L}^{-M-1} \sum_{y=M+1}^{M+L} \delta_{x,-\gamma_1-\gamma_2} \delta_{y,\gamma_2-\gamma_1} \end{aligned}$$

as claimed. □

5.2 Applying an encoded $C\theta$-gate

To implement the controlled phase gate between the mediator qubit and a computational qubit we use some facts about two-particle scattering on a long path. Recall that two indistinguishable particles of momentum k_1 and k_2 initially traveling toward each other will, after scattering, continue to travel as if no interaction occurred, except that the phase of the wave function is modified by the interaction. In general this phase depends on k_1 and k_2 (as well as the interaction $\mathcal{U}$ and the particle statistics). For us, $k_1 = -\pi/2$ and $k_2 = \pi/4$ (moving in opposite directions). We write $e^{i\theta}$ for the phase acquired at these momenta.

5.2.1 Momentum switch

In our scheme we design a subgraph that routes a computational particle and a mediator particle toward each other along a long path only when the two associated qubits are in state $|11\rangle$. This allows us to implement the two-qubit gate

$$\mathrm{C}\theta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\theta} \end{pmatrix}.$$

For some models $\mathrm{C}\theta = \mathrm{CP}$. We show in Section **??** that this holds in the Bose-Hubbard model (where the interaction term is $\mathcal{U}_{ij}(\hat{n}_i, \hat{n}_j) = (U/2)\delta_{i,j}\hat{n}_i(\hat{n}_i - 1)$) when the interaction strength is chosen to be $U = 2 + \sqrt{2}$, since in this case $e^{i\theta} = -i$. For nearest-neighbor interactions with fermions, with $\mathcal{U}_{ij}(\hat{n}_i, \hat{n}_j) = U\delta_{(i,j)\in E(G)}\hat{n}_i\hat{n}_j$, the choice $U = -2 - \sqrt{2}$ gives $e^{i\theta} = i$, so $\mathrm{CP} = (\mathrm{C}\theta)^3$. While tuning the interaction strength makes the CP gate easier to implement, almost any interaction between indistinguishable particles allows for universal computation. We can approximate the required CP gate by repeating the $\mathrm{C}\theta$ gate a times, where $e^{ia\theta} \approx -i$ (which is possible for most values of θ, assuming θ is known [**?**]).

Our strategy requires routing the particles onto a long path. This is done via a subgraph we call the *momentum switch*, as depicted in Figure **??**(a). The S-matrices for this graph at momenta $-\pi/4$ and $-\pi/2$ are

$$S_{\text{switch}}(-\pi/4) = \begin{pmatrix} 0 & 0 & e^{-i\pi/4} \\ 0 & -1 & 0 \\ e^{-i\pi/4} & 0 & 0 \end{pmatrix} \qquad S_{\text{switch}}(-\pi/2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}. \tag{5.18}$$

The momentum switch has perfect transmission between vertices 1 and 3 at momentum $-\pi/4$ and perfect transmission between vertices 2 and 3 at momentum $-\pi/2$. In other words, in the schematic shown in Figure **??**(a), the path a particle follows through the switch depends on its momentum. A particle with momentum $-\pi/2$ follows the double line, while a particle with momentum $-\pi/4$ follows the single line.

The graph used to implement the $\mathrm{C}\theta$ gate has the form shown in Figure **??**(b). We specify the number of vertices on each of the paths in Section **??**. To see why this graph implements a $\mathrm{C}\theta$ gate, consider the movement of two particles as they pass through the graph. If either particle begins in the state $|0_{\text{in}}\rangle$, then it travels along a path to the output without interacting with the second particle. When the computational particle (qubit c in the figure) begins in the state $|1_{\text{in}}\rangle^c$, it is routed downward as it passes through the top momentum switch (following the single line). It travels down the vertical path and then is routed to the right (along the single line) as it passes through the bottom switch. Similarly, when the mediator particle begins in the state $|1_{\text{in}}\rangle^{\text{m}}$, it is routed upward (along the double line) through the vertical path at the bottom switch and then to the right (along the double line) at the top switch. If both particles begin in the state $|1_{\text{in}}\rangle$, then they interact on the vertical path. In this case, as the two particles move past each other, the wave function acquires a phase $e^{i\theta}$ arising from this interaction.

Note that timing is important: the wave packets of the two particles must be on the vertical path at the same time. We achieve this by choosing the number of vertices on each of the segments in the graph appropriately, taking into account the different propagation speeds of the two wave packets (see Section **??** for details).

The Cθ gate is implemented using the graph shown in Figure **??**. In this section we specify the logical input states, the logical output states, the distances X, Z, and W appearing in the figure, and the total evolution time. With these choices, we show that a Cθ gate is applied to the logical states at the end of the time evolution under the quantum walk Hamiltonian (up to error terms that are $\emptyset(L^{-1/4})$). The results of this section pertain to the two-particle Hamiltonian $H^{(2)}_{G'}$ for the graph G' shown in Figure **??**.

The logical input states are

$$|0_{\text{in}}\rangle^c = \frac{1}{\sqrt{L}} \sum_{x=M(-\frac{\pi}{4})+1}^{M(-\frac{\pi}{4})+L} e^{-i\frac{\pi}{4}x}|x,1\rangle \qquad |1_{\text{in}}\rangle^c = \frac{1}{\sqrt{L}} \sum_{x=M(-\frac{\pi}{4})+1}^{M(-\frac{\pi}{4})+L} e^{-i\frac{\pi}{4}x}|x,2\rangle$$

for the computational qubit and

$$|0_{\text{in}}\rangle^{\text{m}} = \frac{1}{\sqrt{L}} \sum_{y=M(-\frac{\pi}{2})+1}^{M(-\frac{\pi}{2})+L} e^{-i\frac{\pi}{2}y}|y,4\rangle \qquad |1_{\text{in}}\rangle^{\text{m}} = \frac{1}{\sqrt{L}} \sum_{y=M(-\frac{\pi}{2})+1}^{M(-\frac{\pi}{2})+L} e^{-i\frac{\pi}{2}y}|y,3\rangle$$

for the mediator qubit. We define symmetrized (or antisymmetrized) logical input states for $a, b \in \{0,1\}$ as

$$\begin{aligned}
|ab_{\text{in}}\rangle^{c,\text{m}} &= \text{Sym}(|a_{\text{in}}\rangle^c|b_{\text{in}}\rangle^{\text{m}}) \\
&= \frac{1}{\sqrt{2}}\left(|a_{\text{in}}\rangle^c|b_{\text{in}}\rangle^{\text{m}} \pm |b_{\text{in}}\rangle^{\text{m}}|a_{\text{in}}\rangle^c\right).
\end{aligned}$$

We choose the distances Z, X, and W from Figure **??** to be

$$Z = 4L \tag{5.19}$$

$$X = d_2 + L + M\left(-\frac{\pi}{2}\right) \tag{5.20}$$

$$W = d_1 + L + M\left(-\frac{\pi}{4}\right) \tag{5.21}$$

where

$$\begin{aligned}
d_1 &= M\left(-\frac{\pi}{4}\right) \\
d_2 &= \left\lceil \frac{5L + 2d_1}{\sqrt{2}} - \frac{5}{2}L \right\rceil.
\end{aligned}$$

With these choices, a wave packet moving with speed $\sqrt{2}$ travels a distance $Z + 2d_1 + L = 5L + 2d_1$ in approximately the same time that a wave packet moving with speed 2 takes to travel a distance $Z + 2d_2 + L = 5L + 2d_2$, since

$$t_{\text{II}} = \frac{5L + 2d_1}{\sqrt{2}} \approx \frac{5L + 2d_2}{2}.$$

We claim that the logical input states evolve into logical output states (defined below) with a phase of $e^{i\theta}$ applied in the case where both particles are in the logical state 1. Specifically,

$$\left\| e^{-iH_{G'}^{(2)}t_{\mathrm{II}}}|00_{\mathrm{in}}\rangle^{c,\mathrm{m}} - |00_{\mathrm{out}}\rangle^{c,\mathrm{m}} \right\| = \emptyset(L^{-1/4}) \tag{5.22}$$

$$\left\| e^{-iH_{G'}^{(2)}t_{\mathrm{II}}}|01_{\mathrm{in}}\rangle^{c,\mathrm{m}} - |01_{\mathrm{out}}\rangle^{c,\mathrm{m}} \right\| = \emptyset(L^{-1/4}) \tag{5.23}$$

$$\left\| e^{-iH_{G'}^{(2)}t_{\mathrm{II}}}|10_{\mathrm{in}}\rangle^{c,\mathrm{m}} - |10_{\mathrm{out}}\rangle^{c,\mathrm{m}} \right\| = \emptyset(L^{-1/4}) \tag{5.24}$$

$$\left\| e^{-iH_{G'}^{(2)}t_{\mathrm{II}}}|11_{\mathrm{in}}\rangle^{c,\mathrm{m}} - e^{i\theta}|11_{\mathrm{out}}\rangle^{c,\mathrm{m}} \right\| = \emptyset(L^{-1/4}) \tag{5.25}$$

where, letting $Q_1 = 2W + Z + 4 - M(-\pi/4) - L$ and $Q_2 = 2X + Z + 6 - M(-\pi/2) - L$,

$$|0_{\mathrm{out}}\rangle^{c} = \frac{e^{-it_{\mathrm{II}}\sqrt{2}}}{\sqrt{L}} \sum_{x=Q_1+1}^{Q_1+L} e^{-i\frac{\pi}{4}x}|x,1\rangle \qquad |1_{\mathrm{out}}\rangle^{c} = \frac{e^{-it_{\mathrm{II}}\sqrt{2}}}{\sqrt{L}} \sum_{x=Q_1+1}^{Q_1+L} e^{-i\frac{\pi}{4}x}|x,2\rangle$$

$$|0_{\mathrm{out}}\rangle^{\mathrm{m}} = \frac{1}{\sqrt{L}} \sum_{y=Q_2+1}^{Q_2+L} e^{-i\frac{\pi}{2}y}|y,4\rangle \qquad |1_{\mathrm{out}}\rangle^{\mathrm{m}} = \frac{1}{\sqrt{L}} \sum_{y=Q_2+1}^{Q_2+L} e^{-i\frac{\pi}{2}y}|y,3\rangle$$

and $|ab_{\mathrm{out}}\rangle^{c,\mathrm{m}} = \mathrm{Sym}\left(|a_{\mathrm{out}}\rangle^{c}|b_{\mathrm{out}}\rangle^{\mathrm{m}}\right)$.

Note that the input states are wave packets located a distance $M(k)$ from the ends of the input paths on the left-hand side of the graph in Figure **??**. Similarly, the output logical states are wave packets located a distance $M(k)$ from the ends of the output paths on the right-hand side.

The first three bounds (5.22), (5.23), and (5.24) are relatively easy to show, since in each case the two particles are supported on disconnected subgraphs and therefore do not interact. In each of these three cases we can simply analyze the propagation of the one-particle starting states through the graph. The symmetrized (or antisymmetrized) starting state then evolves into the symmetrized (or antisymmetrized) tensor product of the two output states.

For example, with input state $|00_{\mathrm{in}}\rangle^{c,\mathrm{m}}$, the evolution of the particle with momentum $-\pi/4$ occurs only on the top path and the evolution of the particle with momentum $-\pi/2$ occurs only on the bottom path. Starting from the initial state $|0_{\mathrm{in}}\rangle^{c}$ and evolving for time t_{II} with the single-particle Hamiltonian for the top path, we obtain the final state

$$|0_{\mathrm{out}}\rangle^{c} + \emptyset(L^{-1/4})$$

using the method of Section **??**. Similarly, starting from the initial state $|0_{\mathrm{in}}\rangle^{\mathrm{m}}$ and evolving for time t_{II} with the single-particle Hamiltonian for the bottom path of the graph we obtain the final state

$$|0_{\mathrm{out}}\rangle^{\mathrm{m}} + \emptyset(L^{-1/4}).$$

Putting these bounds together we get the bound (5.22).

In the case where the input state is $|10_{\mathrm{in}}\rangle^{c,\mathrm{m}}$ (or $|01_{\mathrm{in}}\rangle^{c,\mathrm{m}}$) the single-particle evolution for the particle with momentum $-\pi/4$ (or $-\pi/2$) is slightly more complicated, as in this case the particle moves through the momentum switches and the vertical path. The S-matrix of the momentum switch at the relevant momenta is given by equation (5.18). At momentum $-\pi/4$, the momentum switch has the same S-matrix as a path with 4 vertices (including the input and output vertices). At momentum $-\pi/2$, it has the same S-matrix as a path with 5 vertices (including input and output vertices). Note that our labeling of vertices on the output paths (in Figure **??**) takes this into account. The first vertices on the output paths connected to the momentum switches are labeled $(X+Z+7,3)$ and $(W+Z+5,2)$, respectively, reflecting the fact that a particle with momentum $-\pi/4$ has traveled W vertices on the input path, Z vertices through the middle segment, and has effectively traveled an additional 4 vertices inside the two switches. Similarly, a particle with momentum $-\pi/2$ effectively sees an additional 6 vertices from the two momentum switches.

To get the bound (5.24) we have to analyze the single-particle evolution for the computational particle initialized in the state $|1_{\text{in}}\rangle^c$. We claim that, after time t_{II}, the time-evolved state is

$$|1_{\text{out}}\rangle^c + \emptyset(L^{-1/4}).$$

It is easy to see why this should be the case in light of our discussion above: when scattering at momentum $-\pi/4$, the graph in Figure **??** is equivalent to one where each momentum switch is replaced by a path with 2 internal vertices connecting the relevant input/output vertices.

To make this precise, we use the method described in Section **??** for analyzing scattering through sequences of overlapping graphs using the truncation lemma. Here we should choose subgraphs G_1 and G_2 of the graph G' in Figure **??** that overlap on the vertical path but where each subgraph contains only one of the momentum switches. A convenient choice is to take G_1 to be the subgraph containing the top switch and the paths connected to it (the vertices $(1,2),\ldots,(W,2)$, $(1,5),\ldots,(Z,5)$ and $(X+Z+7,3),\ldots,(2X+Z+6,3)$). Similarly, choose G_2 to be the bottom switch along with the three paths connected to it. The graphs G_1 and G_2 both contain the vertices $(1,5),\ldots,(Z,5)$ along the vertical path. Break up the total evolution time into two intervals $[0,t_\alpha]$ and $[t_\alpha,t_{\text{II}}]$. Choose t_α so that the wave packet, evolved for this time with $H^{(1)}_{G_1}$, travels through the top switch and ends up a distance $\Theta(L)$ from each switch, partway along the vertical path (up to terms bounded as $\emptyset(L^{-1/4})$, as in Section **??**). With this choice, the single-particle evolution with the Hamiltonian for the full graph is approximated by the evolution with $H^{(1)}_{G_1}$ on this time interval (see Section **??**). At time t_α, the particle is outgoing with respect to scattering from the graph G_1, but incoming with respect to G_2. On the interval $[t_\alpha,t_{\text{II}}]$ the time evolution is approximated by evolving the state with $H^{(1)}_{G_2}$. During this time interval the particle travels through the bottom switch onto the final path, and at t_{II} is a distance $M(-\pi/4)$ from the endpoint of the output path. Both switches have the same S-matrix (at momentum $-\pi/4$) as a path of length 4, so this analysis gives the output state $|10_{\text{out}}\rangle^{c,\text{m}}$ up to terms bounded as $\emptyset(L^{-1/4})$, establishing (5.24). For the bound (5.23), we apply a similar analysis to the trajectory of the mediator particle.

The case where the input state is $|11_{\text{in}}\rangle^{c,\text{m}}$ is more involved but proceeds similarly. In this case, to analyze the time evolution we divide the time interval $[0,t_{\text{II}}]$ into three segments $[0,t_A]$, $[t_A,t_B]$, and $[t_B,t_{\text{II}}]$. For each of these three time intervals we choose a subgraph G_A, G_B, G_C of the graph G' in Figure **??** and we approximate the time evolution by evolving with the Hamiltonian on the associated subgraph. We then use the truncation lemma to show that, on each time interval, the evolution generated by the Hamiltonian for the appropriate subgraph approximates the evolution generated by the full Hamiltonian, with error $\varnothing(L^{-1/4})$. Up to these error terms, at times $t = 0$, $t = t_A$, $t = t_B$, and $t = t_{\rm II}$ the time-evolved state

$$e^{-iH^{(2)}_{G'}t}|11_{\rm in}\rangle^{c,{\rm m}}$$

has both particles in square wave packet states, each with support only on L vertices of the graph, as depicted in Figure **??**.

We take G_A to be the subgraph obtained from G' by removing the vertices labeled $(\lceil 1.85L\rceil, 5), \ldots, (\lceil 1.90L\rceil, 5)$ in the vertical path. By removing this interval of consecutive vertices, we disconnect the graph into two components where the initial state $|11_{\rm in}\rangle^{c,{\rm m}}$ has one particle in each component. This could be achieved by removing a single vertex, but instead we remove an interval of approximately $0.05L$ vertices to separate the components of G_A by more than the interaction range C (for sufficiently large L), simplifying our use of the truncation lemma.

We choose $t_A = 3L/2$. Consider the time evolution of the initial state $|11_{\rm in}\rangle^{c,{\rm m}}$ with the two-particle Hamiltonian $H^{(2)}_{G_A}$ for time t_A. The states $|1_{\rm in}\rangle^{c}$ and $|1_{\rm in}\rangle^{\rm m}$ are supported on disconnected components of the graph G_A, so we can analyze the time evolution of the state $|11_{\rm in}\rangle^{c,{\rm m}}$ under $H^{(2)}_{G_A}$ by analyzing two single-particle problems, using the results of Section **??** for each particle. During the interval $[0, t_A]$, each particle passes through one switch, ending up a distance $\Theta(L)$ from the switch that it passed through and $\Theta(L)$ from the vertices that have been removed, as shown in Figure **??**(b) (with error at most $\varnothing(L^{-1/4})$). Up to these error terms, the support of each particle remains at least $N_0 = \Theta(L)$ vertices from the endpoints of the graph, so we can apply the truncation lemma using $H = H^{(2)}_{G'}$, $W = \tilde{H} = H^{(2)}_{G_A}$, $T = t_{\rm A}$, and $\delta = \varnothing(L^{-1/4})$. Here P is the projector onto states where both particles are located at vertices of G_A. We have $PH^{(2)}_{G'}P = H^{(2)}_{G_A}$ since the number of vertices in the removed segment is greater than the interaction range C. Applying the truncation lemma gives

$$\left\| e^{-iH^{(2)}_{G_A}t_A}|11_{\rm in}\rangle^{c,{\rm m}} - e^{-iH^{(2)}_{G'}t_A}|11_{\rm in}\rangle^{c,{\rm m}} \right\| = \varnothing(L^{-1/4}).$$

We approximate the evolution on the interval $[t_A, t_B]$ using the two-particle Hamiltonian $H^{(2)}_{G_B}$, where G_B is the vertical path $(1, 5), \ldots, (Z, 5)$. Using the result of Section **??**, we know that (up to terms bounded as $\varnothing(L^{-1/4})$) the wave packets move with their respective speeds and acquire a phase of $e^{i\theta}$ as they pass each other. We choose $t_B = 5L/2$ so that during the evolution the wave packets have no support on vertices within a distance $\Theta(L)$ from the endpoints of the vertical segment where the graph has been truncated (again up to terms bounded as $\varnothing(L^{-1/4})$). Using $H^{(2)}_{G_B}$ (rather than $H^{(2)}_{G'}$) to evolve the state on this interval, we incur errors bounded as $\varnothing(L^{-1/4})$ (using the truncation lemma with $N_0 = \Theta(L)$, $W = \tilde{H} = H^{(2)}_{G_B}$, $H = H^{(2)}_{G'}$, and $\delta = \varnothing(L^{-1/4})$).

We choose $G_C = G_A$; in the final interval $[t_B, t_{\rm II}]$ we evolve using the Hamiltonian $H^{(2)}_{G_A}$ again, and we use the truncation lemma as we did for the first interval. The initial state is approximated by two wave packets supported on disconnected sections of G_A and the evolution of this initial state reduces to two single-particle scattering problems. During the interval $[t_B, t_{\mathrm{II}}]$, each particle passes through a second switch, and at time t_{II} is a distance $M(k)$ from the end of the appropriate output path.

Our analysis shows that for the input state $|11_{\mathrm{in}}\rangle^{c,\mathrm{m}}$ the only effect of the interaction is to alter the global phase of the final state by a factor of $e^{i\theta}$ relative to the case where no interaction is present, up to error terms bounded as $\O(L^{-1/4})$. This establishes equation (5.25). In Figure **??** we illustrate the movement of the two wave packets through the graph when the initial state is $|11_{\mathrm{in}}\rangle^{c,\mathrm{m}}$.

5.3 Universal Computation

5.3.1 Two-qubit blocks

5.3.2 Combining blocks

5.4 Improvements and Modifications

What about long-range interactions, but where the interactions die off? Additionally, what about error correction?

Chapter 6

Ground energy of quantum walk

To get some flavor for QMA-completeness results.

Now that we have shown the universality of these Quantum Walk Hamiltonians via time evolution, we might want to ask related computational questions about these systems. In particular, once the computational universality of a system is shown, people often ask about the related ground energy problem. The reason for this is that many of these systems that allow for universal computation via time evolution also allow for the encoding of a computation in the ground space, which along with some energy penalties, allow one to show that the ground energy problem is QMA-hard.

The point of this chapter is to give a decent introduction to the flavor of QMA-hardness proofs, as well as providing a QMA-complete problem that might be more accessible to classical computer scientists.

6.1 The ground-energy problem

Essentially, we know that the single-particle quantum walk is governed by the adjacency matrix of the underlying graph. In particular, the Hamiltonian is exactly equal to the adjacency matrix, and thus asking questions about the ground energy of a single-particle quantum walk is simply asking a question about the smallest eigenvalue of a particular adjacency matrix.

However, the Hilbert space on which the quantum walk acts is necessarily exponential in size, with efficiently computable matrix entries. As such, this is a question about very specific types of matrices.

Problem 1 (d-sparse graph eigenvalue problem)**.** Given a d-sparse, row-computable graph G, and two constants $a < b$, is the smallest eigenvalue of $A(G)$ below a or above b, with the guarantee that one of these cases occur.

While this problem is definitely inspired from quantum walks, it actually makes no reference to quantum mechanics.

6.1.1 Containment in QMA

The proof that this problem is in QMAfollows many other such Hamiltonian problems. In particular, this proof strategy works for any system in which we can evolve according to a particular Hamiltonian.

The main idea is to be given a particular state, and use phase estimation to determine the energy of the given state, up to some error. In the case that the smallest eigenvalue of the system is below a, the prover can provide the corresponding eigenvector encoded in a quantum state. The phase estimation algorithm will then (with high probability) find this eigenvalue, and the system will accept. If the smallest eigenvalue is above b, then no matter what state the prover provides, the phase estimation algorithm will project onto one of the eigenstates and determine the corresponding eigenvalue, which will necessarily be above b.

More concretely, we have

6.2 QMA-hardness

The main way that this works is that we will use the well known Kitaev Hamiltonian, with some particular changes so that we get taken to a Hamiltonian of a particular form. Once we have that form, we can easily see that the result we want.

6.2.1 Kitaev Hamiltonian

With the definition of the class QMA, the requirement is that for each input there exists some quantum circuit and some particular input state that the circuit either accepts or rejects. When attempting to prove that a particular Hamiltonian has a similar computational power, we need to construct a "circuit-to-Hamiltonian" map. The predominant (and really only) such map is the so-called Kitaev-Hamiltonian.

In this mapping, we attempt to encode the computation into the ground space of the Hamiltonian, in a similar manner to how the proof that 3-SAT is NP-Hard encodes the entire computation of a nondeterministic Turing Machine. [**TO DO:** *NP-hardness of 3-Sat reference*] However, we run into a problem on how to insure that neighboring time steps are only seperated by a single local unitary. In the classical case we can write down the entire state of the system at each timestep, or else only write down the changes that occur at each time step. In the first case we run into a problem in that information is copied between time steps, which is impossible for a general state by the no-cloning theorem [**TO DO:** *reference no-cloning*] while the second case quickly becomes infeasible as the changes to the quantum state might effect many basis states.

Kitaev worked around this problem by enlarging the Hilbert space on which the circuit acts, by having both a clock and a state register. The computation of the system was then encoded as an entangled state between these two registers. In this way, by having a projection into those states that evolve correctly for a particular time step, we can have a local check for the correctness of evolution.

In particular, if a given circuit $\mathcal{C}$ acts on $\mathbb{C}^{2^m}$ and can be written as $\mathcal{C} = U_T U_{T-1} \cdots U_1$, then the Kitaev Hamiltonian $H_{\mathcal{C}}$ acts on the Hilbert space $\mathbb{C}^{2^m} \otimes \mathbb{C}^{T+1}$, and can be written as

$$H_{\mathcal{C}} = \sum_{t=0}^{T-1} \left(\mathbb{I}_{\mathbb{C}^{2^m}} \otimes |\, t\,\rangle - U_{t+1} \otimes |\, t+1\,\rangle\right)\left(\mathbb{I}_{\mathbb{C}^{2^m}} \otimes \langle\, t\,| - U_{t+1}^{\dagger} \otimes \langle\, t+1\,|\right) = \sum_{t=0}^{T-1} H_t \tag{6.1}$$

Note that each term H_t is a projector off those states of the form

$$|\,\psi\,\rangle \otimes |\,t\,\rangle + U_{t+1}|\,\psi\,\rangle \otimes |\,t+1\,\rangle. \tag{6.2}$$

Hence, we have that the ground state of H_C corresponds to the history states:

$$|\,\psi_{\text{hist}}\,\rangle = \sum_{t=0}^{T} U_t U_{t-1} \cdots U_1 |\,\psi\,\rangle \otimes |\,t\,\rangle. \tag{6.3}$$

These states encode the computation, as for a given initial state $|\,\psi\,\rangle$, the projection onto the time register gives the state of the computation at time t. Note that the energy gap for this Hamiltonian is exactly $1 - \cos(\pi/T)$, as the Hamiltonian is unitarily equivalent to a quantum walk on a line of length T.

With this mapping corresponding to a particular circuit, we can then force the initial state to have a particular form by adding in projectors tensored with a projection onto the $|\,t = 0\rangle$ state, with a similar projection for the requisite form of the final state. Putting everything together we then have a log-local Hamiltonian that will have a polynomial gap depending on whether the initial circuit accepted or rejected.

One can then show that this Hamiltonian will have a low energy eigenvector if and only if the corresponding circuit $\mathcal{C}$ has an accepting input.

6.2.2 Transformation to Adjacency Matrix

While the above prescription works well for the conversion to local-Hamiltonians in the general case, in the situation we are interested in we want all of the non-zero matrix elements to be the same value. As the matrix elements of $H_{\mathcal{C}}$ are related to the matrix values of the unitaries involved in the circuit $\mathcal{C}$, we thus want to force the matrix values of $\mathcal{C}$ to all be of the same form.

To enforce this, we suppose $\mathcal{C}$ implements a unitary

$$U_{\mathcal{C}_x} = U_M \dots U_2 U_1 \tag{6.4}$$

where each U_i acts as

$$\mathcal{G} = \left\{H, HT, (HT)^{\dagger}, (H \otimes \mathbb{I})\,\text{CNOT}\right\} \tag{6.5}$$

on some qubits, and the identity on the rest.

Note that this gate set is universal, as we can easily simulate the gate set $\{H, T, \text{CNOT}\}$ with gates from $\mathcal{G}$ since $H^2 = \mathbb{I}$ and we can thus cancel the H terms before the interesting portion of the gates. Further, each non-zero matrix element of these unitaries has norm $2^{-1/2}$, as we wanted.

However, when we look at one of the local terms in the Hamiltonian, we find that not all of the matrix elements have the same norm. In particular, we find that

$$H_t = \left(\mathbb{I}_{\mathbb{C}^{2^m}} \otimes |\,t\,\rangle - U_{t+1} \otimes |\,t+1\,\rangle\right)\left(\mathbb{I}_{\mathbb{C}^{2^m}} \otimes \langle\,t\,| - U_{t+1}^{\dagger} \otimes \langle\,t+1\,|\right) \tag{6.6}$$

$$= \mathbb{I}_{\mathbb{C}^{2^m}} \otimes \left(|\,t\,\rangle\langle\,t\,| + |\,t+1\,\rangle\langle\,t+1\,|\right) - \left(U_{t+1} \otimes |\,t+1\,\rangle\langle\,t\,| + U_{t+1}^{\dagger} \otimes |\,t\,\rangle\langle\,t+1\,|\right). \tag{6.7}$$

While each off-diagonal term is either zero or has norm $2^{-1/2}$ in (6.7), the diagonal terms have norm 1. When each term is summed, we almost have that the sum of the diagonal terms are proportional to the identity, but unfortunately the boundary terms (with $t = 0$ or $t = T$) are only involved in one unitary. However, this problem can be avoided by having circular time, in which we both compute and uncompute the comptutation. With this, each timestep is involved in exactly two local terms, and thus the diagonal term is proportional to the identity.

With this, it will be convenient to consider

$$U_{\mathcal{C}}^{\dagger} U_{\mathcal{C}} = W_{2M} \ldots W_2 W_1 \tag{6.8}$$

where

$$W_t = \begin{cases} U_t & 1 \le t \le M \\ U_{2M+1-t}^{\dagger} & M+1 \le t \le 2M. \end{cases} \tag{6.9}$$

As in Section 6.2.1 we start with a version of the Feynman-Kitaev Hamiltonian (with a different norm) [?, ?] acting on the Hilbert space $\mathcal{H}_{\text{comp}} \otimes \mathcal{H}_{\text{clock}}$ where $\mathcal{H}_{\text{comp}} = (\mathbb{C}^2)^{\otimes m}$ is an m-qubit computational register and $\mathcal{H}_{\text{clock}} = \mathbb{C}^{2M}$ is a $2M$-level register with periodic boundary conditions (i.e., we let $|2M+1\rangle = |1\rangle$). However, we then subtract a term proportional to the identity, which yields the Hamiltonian

$$H_{\mathcal{C}} = -\sqrt{2} \sum_{t=1}^{2M} \left(W_t^{\dagger} \otimes |t\rangle\langle t+1| + W_t \otimes |t+1\rangle\langle t| \right). \tag{6.10}$$

Note that

$$V^{\dagger} H_{\mathcal{C}} V = -\sqrt{2} \sum_{t=1}^{2M} \left(\mathbb{I} \otimes |t\rangle\langle t+1| + \mathbb{I} \otimes |t+1\rangle\langle t| \right) \tag{6.11}$$

where

$$V = \sum_{t=1}^{2M} \left(\prod_{j=t-1}^{1} W_j \right) \otimes |t\rangle\langle t| \tag{6.12}$$

and $W_0 = 1$. Since V is unitary, the eigenvalues of H_x are the same as the eigenvalues of (6.11), namely

$$-2\sqrt{2} \cos\left(\frac{\pi \ell}{M}\right) \tag{6.13}$$

for $\ell = 0, \ldots, 2M-1$. The ground energy of (6.11) is $-2\sqrt{2}$ and its ground space is spanned by

$$|\phi\rangle \frac{1}{\sqrt{2M}} \sum_{j=1}^{2M} |t\rangle, \quad |\phi\rangle \in \Lambda \tag{6.14}$$

where Λ is any orthonormal basis for $\mathcal{H}_{\text{comp}}$. A basis for the ground space of H_x is therefore

$$V\left(|\phi\rangle \frac{1}{\sqrt{2M}} \sum_{j=1}^{2M} |t\rangle\right) = \frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} W_{t-1} W_{t-2} \ldots W_1 |\phi\rangle |t\rangle \tag{6.15}$$

where $|\phi\rangle \in \Lambda$. The first excited energy of H_x is

$$\eta = -2\sqrt{2} \cos\left(\frac{\pi}{M}\right) \tag{6.16}$$

and the gap between ground and first excited energies is lower bounded as

$$\eta + 2\sqrt{2} \geq \sqrt{2} \frac{\pi^2}{M^2} \tag{6.17}$$

(using the fact that $1 - \cos(x) \leq \frac{x^2}{2}$).

The universal set $\mathcal{G}$ is chosen so that each gate has nonzero entries that are integer powers of $\omega = e^{i\frac{\pi}{4}}$. Correspondingly, the nonzero standard basis matrix elements of $H_{\mathcal{C}}$ are also integer powers of $\omega = e^{i\frac{\pi}{4}}$. We consider the 8×8 shift operator

$$S = \sum_{j=0}^{7} |j + 1 \bmod 8\rangle\langle j| \tag{6.18}$$

and note that ω is an eigenvalue of S with eigenvector

$$|\omega\rangle = \frac{1}{\sqrt{8}} \sum_{j=0}^{7} \omega^{-j} |j\rangle. \tag{6.19}$$

We modify $H_{\mathcal{C}}$ as follows. For each operator $-\sqrt{2}H$, $-\sqrt{2}HT$, $-\sqrt{2}(HT)^{\dagger}$, or $-\sqrt{2}\,(H \otimes \mathbb{I})\,\text{CNOT}$ appearing in equation (6.10), define another operator that acts on $\mathbb{C}^2 \otimes \mathbb{C}^8$ or $\mathbb{C}^4 \otimes \mathbb{C}^8$ (as appropriate) by replacing nonzero matrix elements with powers of the operator S:

$$\omega^k \mapsto S^k.$$

Matrix elements that are zero are mapped to the 8×8 all-zeroes matrix. Write $B(W)$ for the operators obtained by making this replacement, e.g.,

$$-\sqrt{2}HT = \begin{pmatrix} \omega^4 & \omega^5 \\ \omega^4 & \omega \end{pmatrix} \mapsto B(HT) = \begin{pmatrix} S^4 & S^5 \\ S^4 & S \end{pmatrix}.$$

Adjoining an 8-level ancilla as a third register and making this replacement in equation (7.12) gives

$$H_{\text{prop}} = \sum_{t=1}^{2M} \left(B(W_t)_{13}^{\dagger} \otimes |t\rangle\langle t+1|_2 + B(W_t)_{13} \otimes |t+1\rangle\langle t|_2 \right) \tag{6.20}$$

which is a symmetric 0-1 matrix (the subscripts indicate which registers the operators act on). Note that H_{prop} commutes with S (acting on the 8-level ancilla) and therefore is block diagonal with eight sectors. In the sector where S has eigenvalue ω, H_{prop} is identical to the Hamiltonian $H_{\mathcal{C}}$ that we started with (see equation (6.10)). There is also a sector (where S has eigenvalue ω^*) where the Hamiltonian is the element-wise complex conjugate of $H_{\mathcal{C}}$. We will add a term to H_{prop} that introduces an energy penalty for states in any of the other six sectors, ensuring that none of these states lie in the ground space.

To see what kind of energy penalty is needed, we lower bound the eigenvalues of H_{prop}. Note that for each $W \in \mathcal{G}$, $B(W)$ contains at most 2 ones in each row or column. Looking at equation (6.20) and using this fact, we see that each row and each column of H_{prop} contains at most four ones (with the remaining entries all zero). Therefore $\|H_{\text{prop}}\| \leq 4$, so every eigenvalue of H_{prop} is at least -4.

The matrix A_x associated with the circuit $\mathcal{C}_x$ acts on the Hilbert space

$$\mathcal{H}_{\text{comp}} \otimes \mathcal{H}_{\text{clock}} \otimes \mathcal{H}_{\text{anc}} \tag{6.21}$$

where $\mathcal{H}_{\text{anc}} = \mathbb{C}^8$ holds the 8-level ancilla. We define

$$A_x = H_{\text{prop}} + H_{\text{penalty}} + H_{\text{input}} + H_{\text{output}} \tag{6.22}$$

where

$$H_{\text{penalty}} = \mathbb{I} \otimes \mathbb{I} \otimes \left(S^3 + S^4 + S^5\right) \tag{6.23}$$

is the penalty ensuring that the ancilla register holds either $|\omega\rangle$ or $|\omega^*\rangle$ and the terms

$$H_{\text{input}} = \sum_{j=n_{\text{input}}+1}^{n} |1\rangle\langle 1|_j \otimes |1\rangle\langle 1| \otimes \mathbb{I}$$

$$H_{\text{output}} = |0\rangle\langle 0|_{\text{output}} \otimes |M+1\rangle\langle M+1| \otimes \mathbb{I}$$

ensure that the ancilla qubits are initialized in the state $|0\rangle$ when $t = 1$ and that the output qubit is in the state $|1\rangle\langle 1|$ when the circuit $\mathcal{C}_x$ has been applied (i.e., at time $t = M + 1$). Observe that A_x is a symmetric 0-1 matrix.

Now consider the ground space of the first two terms $H_{\text{prop}} + H_{\text{penalty}}$ in (6.22). Note that $[H_{\text{prop}}, H_{\text{penalty}}] = 0$, so these operators can be simultaneously diagonalized. Furthermore, H_{penalty} has smallest eigenvalue $-1-\sqrt{2}$, with eigenspace spanned by $|\omega\rangle$ and $|\omega^*\rangle$. One can also easily confirm that the first excited energy of H_{penalty} is -1.

The ground space of $H_{\text{prop}} + H_{\text{penalty}}$ lives in the sector where H_{penalty} has minimal eigenvalue $-1-\sqrt{2}$. To see this, note that within this sector H_{prop} has the same eigenvalues as H_x, and therefore has lowest eigenvalue $-2\sqrt{2}$. The minimum eigenvalue e_1 of $H_{\text{prop}} + H_{\text{penalty}}$ in this sector is

$$e_1 = -2\sqrt{2} + \left(-1 - \sqrt{2}\right) = -1 - 3\sqrt{2} = -5.24\ldots, \tag{6.24}$$

whereas in any other sector H_{penalty} has eigenvalue at least -1 and (using the fact that $H_{\text{prop}} \geq -4$) the minimum eigenvalue of $H_{\text{prop}} + H_{\text{penalty}}$ is at least -5. Thus, an orthonormal basis for the ground space of $H_{\text{prop}} + H_{\text{penalty}}$ is furnished by the states

$$\frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} W_{t-1} W_{t-2} \ldots W_1 |\phi\rangle |t\rangle |\omega\rangle \tag{6.25}$$

$$\frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} (W_{t-1} W_{t-2} \ldots W_1)^* |\phi^*\rangle |t\rangle |\omega^*\rangle \tag{6.26}$$

where $|\phi\rangle$ ranges over the basis Λ for $\mathcal{H}_{\text{comp}}$ and $*$ denotes (elementwise) complex conjugation.

At this point, we then have a symmetric 0-1 matrix whose ground-space is spanned by history states. While we have not yet shown that determining the ground energy of this matrix is QMA-hard, this graph is the result of our circuit-to-graph mapping.

6.2.3 Upper bound on the smallest eigenvalue for yes instances

Suppose x is a yes instance; then there exists some n_{input}-qubit state $|\psi_{\text{input}}\rangle$ satisfying $\text{AP}\left(\mathcal{C}_x, |\psi_{\text{input}}\rangle\right) \geq 1 - \frac{1}{2^{|x|}}$. Let

$$|\text{wit}\rangle = \frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} W_{t-1}W_{t-2}\ldots W_1 \left(|\psi_{\text{input}}\rangle|0\rangle^{\otimes n-n_{\text{input}}}\right)|t\rangle|\omega\rangle \tag{6.27}$$

and note that this state is in the e_1-energy ground space of $H_{\text{prop}} + H_{\text{penalty}}$ (since it has the form (6.25)). One can also directly verify that $|\text{wit}\rangle$ has zero energy for H_{input}. Thus

$$\begin{aligned}
\langle\text{wit}|A_x|\text{wit}\rangle &= e_1 + \langle\text{wit}|H_{\text{output}}|\text{wit}\rangle \\
&= e_1 + \frac{1}{2M}\langle\psi_{\text{input}}|\langle 0|^{\otimes n-n_{\text{input}}} U_{\mathcal{C}_x}^{\dagger}|0\rangle\langle 0|_{\text{output}} U_{\mathcal{C}_x}|\psi_{\text{input}}\rangle|0\rangle^{\otimes n-n_{\text{input}}} \\
&= e_1 + \frac{1}{2M}\left(1 - \text{AP}(\mathcal{C}_x, |\psi_{\text{input}}\rangle)\right) \\
&\leq e_1 + \frac{1}{2M}\frac{1}{2^{|x|}}.
\end{aligned}$$

6.2.4 Lower bound on the smallest eigenvalue for no instances

Now suppose x is a no instance. Then the verification circuit $\mathcal{C}_x$ has acceptance probability $\text{AP}\left(\mathcal{C}_x, |\psi\rangle\right) \leq \frac{1}{3}$ for all n_{input}-qubit input states $|\psi\rangle$.

We backtrack slightly to obtain bounds on the eigenvalue gaps of the Hamiltonians $H_{\text{prop}}+H_{\text{penalty}}$ and $H_{\text{prop}} + H_{\text{penalty}} + H_{\text{input}}$. We begin by showing that the energy gap of $H_{\text{prop}} + H_{\text{penalty}}$ is at least an inverse polynomial function of M. Subtracting a constant equal to the ground energy times the identity matrix sets the smallest eigenvalue to zero, and the smallest nonzero eigenvalue satisfies

$$\gamma(H_{\text{prop}} + H_{\text{penalty}} - e_1 \cdot \mathbb{I}) \geq \min\left\{\sqrt{2}\frac{\pi^2}{M^2}, -5 - e_1\right\} \geq \frac{1}{5M^2}. \tag{6.28}$$

since $-5 - e_1 \approx 0.24\ldots > \frac{1}{5}$. The first inequality above follows from the fact that every eigenvalue of H_{prop} in the range $[e_1, -5)$ is also an eigenvalue of H_x (as discussed above) and the bound (6.17) on the energy gap of H_x.

Now use the Nullspace Projection Lemma (Lemma **??**) with

$$H_A = H_{\text{prop}} + H_{\text{penalty}} - e_1 \cdot \mathbb{I} \qquad H_B = H_{\text{input}}. \tag{6.29}$$

Note that H_A and H_B are positive semidefinite. Let S_A be the ground space of H_A and consider the restriction $H_B|_{S_A}$. Here it is convenient to use the basis for S_A given by (6.25) and (6.26) with $|\phi\rangle$ ranging over the computational basis states of n qubits. In this basis, $H_B|_{S_A}$ is diagonal with all diagonal entries equal to $\frac{1}{2M}$ times an integer, so $\gamma(H_B|_{S_A}) \geq \frac{1}{2M}$. We also have $\gamma(H_A) \geq \frac{1}{5M^2}$ from equation (6.28), and clearly $\|H_B\| \leq n$. Thus Lemma ?? gives

$$\gamma(H_{\text{prop}} + H_{\text{penalty}} + H_{\text{input}} - e_1 \cdot \mathbb{I}) \geq \frac{\left(\frac{1}{5M^2}\right)\left(\frac{1}{2M}\right)}{\frac{1}{5M^2} + \frac{1}{2M} + n} \geq \frac{1}{10M^3\,(1+n)} \geq \frac{1}{20M^3 n}. \tag{6.30}$$

Now consider adding the final term H_{output}. We use Lemma ?? again, now setting

$$H_A = H_{\text{prop}} + H_{\text{penalty}} + H_{\text{input}} - e_1 \cdot \mathbb{I} \qquad H_B = H_{\text{output}}. \tag{6.31}$$

Let S_A be the ground space of H_A. Note that it is spanned by states of the form (6.25) and (6.26) where $|\phi\rangle = |\psi\rangle|0\rangle^{\otimes n-n_{\text{input}}}$ and $|\psi\rangle$ ranges over any orthonormal basis of the n_{input}-qubit input register. The restriction $H_B|_{S_A}$ is block diagonal, with one block for states of the form

$$\frac{1}{\sqrt{2M}}\sum_{t=1}^{2M} W_{t-1}W_{t-2}\ldots W_1\left(|\psi\rangle|0\rangle^{\otimes n-n_{\text{input}}}\right)|t\rangle|\omega\rangle \tag{6.32}$$

and another block for states of the form

$$\frac{1}{\sqrt{2M}}\sum_{t=1}^{2M} (W_{t-1}W_{t-2}\ldots W_1)^*\left(|\psi\rangle^*|0\rangle^{\otimes n-n_{\text{input}}}\right)|t\rangle|\omega^*\rangle. \tag{6.33}$$

We now show that the minimum eigenvalue of $H_B|_{S_A}$ is nonzero, and we lower bound it. We consider the two blocks separately. By linearity, every state in the first block can be written in the form (6.32) for some state $|\psi\rangle$. Thus the minimum eigenvalue within this block is the minimum expectation of H_{output} in a state (6.32), where the minimum is taken over all n_{input}-qubit states $|\psi\rangle$. This is equal to

$$\min_{|\psi\rangle}\frac{1}{2M}\left(1 - \text{AP}(\mathcal{C}_x, |\psi\rangle)\right) \geq \frac{1}{3M} \tag{6.34}$$

where we used the fact that $\text{AP}\left(\mathcal{C}_x, |\psi\rangle\right) \leq \frac{1}{3}$ for all $|\psi\rangle$. Likewise, every state in the second block can be written as (6.33) for some state $|\psi\rangle$, and the minimum eigenvalue within this block is

$$\min_{|\psi\rangle}\frac{1}{2M}\left(1 - \text{AP}(\mathcal{C}_x, |\psi\rangle)^*\right) \geq \frac{1}{3M} \tag{6.35}$$

(since $\text{AP}(\mathcal{C}_x, |\psi\rangle)^* = \text{AP}(\mathcal{C}_x, |\psi\rangle) \leq \frac{1}{3}$). Thus we see that $H_B|_{S_A}$ has an empty nullspace, so its smallest eigenvalue is equal to its smallest nonzero eigenvalue, namely

$$\gamma(H_B|_{S_A}) \geq \frac{1}{3M}. \tag{6.36}$$

Now applying Lemma ?? using this bound, the fact that $\|H_B\| = 1$, and the fact that $\gamma(H_A) \geq \frac{1}{20M^3 n}$ (from equation (6.30)), we get

$$\gamma(A_x - e_1 \cdot \mathbb{I}) \geq \frac{\frac{1}{60M^4 n}}{\frac{1}{20M^3 n} + \frac{1}{3M} + 1} \geq \frac{1}{120M^4 n}. \tag{6.37}$$

Since $H_B|_{S_A}$ has an empty nullspace, $A_x - e_1 \cdot \mathbb{I}$ has an empty nullspace, and this is a lower bound on its smallest eigenvalue.

6.3 Extensions and Discussion

While this result is interesting in its own right, as it shows that finding the ground energy of a sparse, row-computable matrix is QMA-complete, perhaps the most interesting result is that nothing particularly quantum is involved in the definition of the problem. In particular, the only condition we have on the matrix is that it is sparse, and row-computable. This condition might allow for a more natural understanding for more classically-minded computer scientists, as a QMA-complete problem could be stated without having to delve into any quantum computing.

As an additional problem, since the circuit-to-Hamiltonian map creates a 7-regular, simple graph, one might wonder if the removal of these conditions are necessary when the boundary terms are added. This is obviously going to be necessary, as otherwise we would have that determining the lowest eigenvalue of a Laplacian is QMA-complete, but it is a well known fact that the smallest eigenvalue of a Laplacian is zero.

[**TO DO:** *can I use the same techniques as the self-loop removal to remove self-loops from this system?*]

[**TO DO:** *Write more*]

Chapter 7

Ground energy of multi-particle quantum walk

With our proof that the ground state problem for a single-particle quantum walk is QMA-complete, we would now like to examine the corresponding problem for the multi-particle quantum walk. The similarities between the two systems make us expect that very similar results will hold for the multi-particle case, but we will again need to examine the problem in a lot of detail.

In particular, the QMA-completeness for the single particle walk was relatively straightforward, in that there is really only one particle to deal with. Because of this, we understand the dynamics and can exactly analyze the system on which things interact, leading to exact solutions for the energies of the resulting Hamiltonian. With the MPQW, a full analysis is currently beyond our knowledge, and our universality construction relied on a reduction to the cases with at most two interacting particles. In order to show that finding the ground energy of a MPQW is QMA-complete using our techniques, we'd need to again reduce to the case of a small number of particles.

To make this reduction, we will show that the problem is QMA-hard when restricted to the problem where the interaction term adds (almost) no energy to the ground state, so that the ground state is contained within the span of single-particle states that don't overlap. With this restriction, we will still have correlations between many particles, but we will be able to analyze the correlations and determine the corresponding ground energy.

7.1 MPQW Hamiltonian ground-energy problem

In order to make things precise, we will fix a particular finite-range interaction, and show that with this fixed interaction, the resulting question is QMA-complete to solve. In particular let $\mathcal{U}$ be an interaction with finite support and no negative coefficients. For a particular graph G, we can then define a Hamiltonian on such a graph as [**TO DO:** *find a correct way to define* $\mathcal{U}$]

$$H_{f,G} = \sum_{(i,j)\in E(G)} a_i a_j + a_j a_i + \sum_{i,j\in V(G)} U_{d(i,j)}(n_i, n_j) = H_{G,\text{move}} + H_{G,\text{int}}. \tag{7.1}$$

Note that because of the positivity restrictions placed on $\mathcal{U}$, we have that $H_{G,\text{int}}$ is positive semi-definite, and thus the ground energy of $H_{f,G}$ is at least the ground energy of $H_{G,\text{move}}$.

With this particular interaction, we can then construct the corresponding problem.

Note that these Hamiltonians actually act on an infinite dimensional Hilbert space, in that the number of particles is unbounded. In order to reduce the complexity of these problems to a reasonable amount, we restrict our attention to a particular number of particles. Once again, as each term in the Hamiltonian preserves the number of particles, we have that $H_{\mathcal{U},G}$ decomposes into blocks with a particular particle number, and we represent these blocks as $\overline{H}_{\mathcal{U},G}^{N}$.

Problem 2 ($\mathcal{U}$-interaction MPQW Hamiltonion)**.** Given as input a K-vertex graph G, a number of particles N, a real number c, and a precision parameter $\epsilon = 1/T$, where the positive integers N and T are given in unary, and the graph G is given as its adjacency matrix (a $K \times K$ symmetric 0-1 matrix), the $\mathcal{U}$-interaction MPQW Hamiltonian problem is to determine whether the smallest eigenvalue of $\overline{H}_{\mathcal{U},G}^{N}$ is at most c or is at least $c + \epsilon$, with a promise that one of these two cases hold.

7.1.1 MPQW Hamiltonian is contained in QMA

To prove that $\mathcal{U}$-interaction MPQW Hamiltonian problem is contained in QMA, we provide a verification algorithm satisfying the requirements of Definition **??**. In the Definition this algorithm is specified by a circuit involving only one measurement of the output qubit at the end of the computation. The procedure we describe below, which contains intermediate measurements in the computational basis, can be converted into a verification circuit of the desired form by standard techniques.

We are given an instance specified by G, N, c, and ϵ. We are also given an input state $|\phi\rangle$ of n_{input} qubits, where $n_{\text{input}} = \lceil \log_2 D_N \rceil$ and D_N is the dimension of $\mathcal{Z}_N(G)$ as given in equation (**??**). Note, using the inequality $\binom{a}{b} \leq a^b$ in equation (**??**), that $n_{\text{input}} = \mathcal{O}(K \log(N + K))$, where $K = |V|$ is the number of vertices in the graph G. We embed $\mathcal{Z}_N(G)$ into the space of n_{input} qubits straightforwardly as the subspace spanned by the first D_N standard basis vectors (with lexicographic ordering, say). The first step of the verification procedure is to measure the projector onto this space $\mathcal{Z}_N(G)$. If the measurement outcome is 1 then the resulting state $|\phi'\rangle$ is in $\mathcal{Z}_N(G)$ and we continue; otherwise we reject.

In the second step of the verification procedure, the goal is to measure $\bar{H}_G^N$ in the state $|\phi'\rangle$. The Hamiltonian $\bar{H}_G^N$ is sparse and efficiently row-computable, with norm

$$\left\|\bar{H}_G^N\right\| \leq \left\|H_G^N\right\| \leq N \left\|A(G)\right\| + \left\|\sum_{k \in V} \hat{n}_k \left(\hat{n}_k - 1\right)\right\| \leq NK + N^2.$$

We use phase estimation (see for example [**?**]) to estimate the energy of $|\phi'\rangle$, using sparse Hamiltonian simulation [**?**] to approximate evolution according to $\bar{H}_G^N$. We choose the parameters of the phase estimation so that, with probability at least $\frac{2}{3}$, it produces an approximation E of the energy with error at most $\frac{\epsilon}{4}$. This can be done in time $\text{poly}(N, K, \frac{1}{\epsilon})$. If $E \leq c + \frac{\epsilon}{2}$ then we accept; otherwise we reject.

We now show that this verification procedure satisfies the completeness and soundness requirements of Definition **??**. For a yes instance, an eigenvector of $\bar{H}_G^N$ with eigenvalue $e \leq c$ is accepted by this procedure as long as the energy E computed in the phase estimation step has the desired precision. To see this, note that we measure $|E - e| \leq \frac{\epsilon}{4}$, and hence $E \leq c + \frac{\epsilon}{4}$, with probability at least $\frac{2}{3}$. For a no instance, write $|\phi'\rangle \in \mathcal{Z}_N(G)$ for a state obtained after passing the first step. The value E computed by the subsequent phase estimation step satisfies $E \geq c + \frac{3\epsilon}{4}$ with probability at least $\frac{2}{3}$, in which case the state is rejected. From this we see that the probability of accepting a no instance is at most $\frac{1}{3}$.

7.1.2 Frustration-free

While showing that this problem is contained in QMAis relatively easy, in our proof of QMA-hardness we will want to impose additional structure on the problem. In particular, we will want the problem to have the extra promise that if the particular instance is a yes instance, then the interaction term will essentially add no energy to the ground state. In particular, we will want the ground state of the system to be a ground state for each term in the Hamilonian individually, which is usually a statement that the Hamiltonian is frustration-free.

The reason that this helps us is that it actually allows us to determine the actual ground energies of various Hamiltonians, and lets us convert the problem to one of adding positive semi-definite matrices. This allows us to use our Nullspace Projection Lemma (Lemma **??**), and give strong bounds on the resulting eigenvalue gaps. Additionally, the guarantee that certain Hamilonians are frustration-free will allow us to give some additional results on various spin systems.

[**TO DO:** *does this work for both bosons and fermions?. I think it will, but I'm not sure. It might not be worth it to discuss fermions right now.*]

With all of this, let G be a graph, and let us assume that the interaction is $\mathcal{U}$. If we then restrict to the N-particle sector, we have that the Hamiltonian is given by

$$H_{\mathcal{U},G}^N = \sum_{(i,j)\in E(G)} a_i^\dagger a_j + a_j^\dagger a_i + \sum_{i,j\in V(G)} \mathcal{U}_{d(i,j)}(n_i, n_j) \tag{7.2}$$

$$= \sum_{w=1}^N A(G)^{(w)} + \sum_{i,j\in V(G)} \mathcal{U}_{d(i,j)}(\hat{n}_i, \hat{n}_j) \tag{7.3}$$

where

$$\hat{n}_i = \sum_{w=1}^N |\, i\,\rangle\langle\, i\,|^{(w)}. \tag{7.4}$$

While $H_{\mathcal{U},G}^N$ acts on the entire $|V|^N$ dimensional system of distinguishable particles, we want to deal with indistinguishable particles (and in particular bosonic particles). As such, we will want to look at the restriction of $H_{\mathcal{U},G}^N$ to the bosonic subspace:

$$\overline{H}_{\mathcal{U},G}^N := H_{\mathcal{U},G}^N\big|_{\mathcal{Z}_N(G)} \tag{7.5}$$

[**TO DO:** *check boson/fermion*]

At this point, it will be extremely useful to add a term proportional to the identity in order to make a positive semidefinite operator. In particular, if we let $\mu(G)$ be the smallest eigenvalue of $A(G)$, we can consider

$$H_{\mathcal{U}}(G,N) = \overline{H}^{n}_{\mathcal{U},G} - N\mu(G) \tag{7.6}$$

which is a positive-semidefinite matrix. Additionally, as $\mu(G)$ can be efficiently computed using a classical polynomial-time algorithm, we have that the complexity of approximating the ground energy of $H_{\mathcal{U}}(G,N)$ is equivalent to the complexity of approximating the ground energy of $\overline{H}^{N}_{\mathcal{U},G}$.

We shall write

$$0 \leq \lambda_N^1(G) \leq \lambda_N^2(G) \leq \cdots \leq \lambda_N^{D_N}(G) \tag{7.7}$$

for the eigenvalues of $H_{\mathcal{U}}(G,N)$ and $\{|\,\lambda_N^j(G)\,\rangle\}$ for the associated eigenvectors.

Note that when $\lambda_N^1(G) = 1$, the ground energy of the N-particle MPQW Hamiltonian $\overline{H}^{N}_{\mathcal{U},G}$ is equal to N times the single-particle ground energy $\mu(G)$. In this case, we say that the N-particle MPQW Hamiltonian is frustration free, as the ground state minimizes both the movement term and the interaction term. We also define frustration freeness for N-particle states.

Definition 6 (Frustration-free state)**.** If $|\,\psi\,\rangle \in \mathcal{Z}_N(G)$ satisfies $H_{\mathcal{U}}(G,N)|\,\psi\,\rangle = 0$, then we say that $|\,\psi\,\rangle$ is an N-particle frustration-free state for $\mathcal{U}$ on G.

7.1.2.1 Basic properties

We now give some basic properties of $H_{\mathcal{U}}(G,N)$. In particular we will want to understand how the eigenvalues of the Hamiltonian change when we increase the number of particles, as well as understand such a system when looking at many disconnected copies of graphs.

Lemma 11. *For all $N > 1$, $\lambda_{N+1}^1(G) \geq \lambda_N^1(G)$.*

Proof. [**TO DO:** *Fix this for an arbitrary interaciton*] Let $\widehat{n}_i^N$ be the number operator (**??**) defined in the N-particle space and let $\widehat{n}_i^{N+1}$ be the corresponding operator in the $(N+1)$-particle space. Note that

$$\widehat{n}_i^{N+1} = \widehat{n}_i^N \otimes \mathbb{I} + |i\rangle\langle i|^{(N+1)} \geq \widehat{n}_i^N \otimes \mathbb{I}.$$

Using this and the fact that $A(G) \geq \mu(G)$, we get

$$H_G^{N+1} - (N+1)\,\mu(G) \geq \left(H_G^N - N\mu(G)\right) \otimes \mathbb{I}.$$

Hence

$$\begin{aligned}
\lambda_{N+1}^1(G) &= \min_{|\psi\rangle \in \mathcal{Z}_{N+1}(G):\ \langle\psi|\psi\rangle=1} \langle\psi|H_G^{N+1} - (N+1)\,\mu(G)|\psi\rangle \\
&\geq \min_{|\psi\rangle \in \mathcal{Z}_N(G)\otimes\mathbb{C}^{|V|}:\ \langle\psi|\psi\rangle=1} \langle\psi|\left(H_G^N - N\mu(G)\right)\otimes\mathbb{I}|\psi\rangle \\
&= \lambda_N^1(G)
\end{aligned}$$

(using the fact that $\mathcal{Z}_{N+1}(G) \subset \mathcal{Z}_N(G) \otimes \mathbb{C}^{|V|}$). ∎

We will encounter graphs G with more than one component. In the cases of interest, the smallest eigenvalue of the adjacency matrix for each component is the same. The following Lemma shows that the eigenvalues of $H(G,N)$ on such a graph can be written as sums of eigenvalues for the components. In this Lemma (and throughout the paper), we let $[k]=\{1,2,\ldots,k\}$.

Lemma 12. *Suppose $G=\bigcup_{i=1}^{k} G_i$ with $\mu(G_1)=\mu(G_2)=\cdots=\mu(G_k)$. The eigenvalues of $H(G,N)$ are*

$$\sum_{i\in[k]:\ N_i\neq 0} \lambda_{N_i}^{y_i}(G_i)$$

where $N_1,\ldots,N_k\in\{0,1,2,\ldots\}$ with $\sum_i N_i=N$ and $y_i\in[D_{N_i}]$. The corresponding eigenvectors are (up to normalization)

$$\mathrm{Sym}\left(\prod_{i\in[k]:\ N_i\neq 0} |\lambda_{N_i}^{y_i}(G_i)\rangle\right). \tag{7.8}$$

Proof. Recall that the action of $H_G-N\mu(G)$ on the Hilbert space (**??**) is the same as the action of $H(G,N)$ on the Hilbert space $\mathcal{Z}_N(G)$. States in these Hilbert spaces are identified via the mapping described in equation (**??**). It is convenient to prove the Lemma by working with the second-quantized Hamiltonian H_G. We then translate our results into the first-quantized picture to obtain the stated claims.

For a graph with k components, equation (**??**) gives

$$H_G=\sum_{i=1}^{k} H_{G_i} \tag{7.9}$$

where $[H_{G_i},H_{G_j}]=0$. Label each vertex of G by (a,b) where $b\in[k]$ and $a\in[|V_b|]$, where V_b is the vertex set of the component G_b. An occupation number basis state (**??**) can be written

$$|l_{1,1},\ldots,l_{|V_1|,1}\rangle|l_{1,2},\ldots,l_{|V_2|,2}\rangle\ldots|l_{1,k},\ldots,l_{|V_k|,k}\rangle. \tag{7.10}$$

The Hamiltonian $H_G-N\mu(G)$ conserves the number of particles N_b in each component b. Within the sector corresponding to a given set $N_1,\ldots,N_k$ with $\sum_{i\in[k]}N_i=N$, we have

$$\begin{aligned}
&(H_G-N\mu(G))\,|l_{1,1},\ldots,l_{|V_1|,1}\rangle|l_{1,2},\ldots,l_{|V_2|,2}\rangle\ldots|l_{1,k},\ldots,l_{|V_k|,k}\rangle\\
&\quad=\big(H_{G_1}-N_1\mu(G_1)|l_{1,1},\ldots,l_{|V_1|,1}\rangle\big)|l_{1,2},\ldots,l_{|V_2|,2}\rangle\ldots|l_{1,k},\ldots,l_{|V_k|,k}\rangle\\
&\qquad+|l_{1,1},\ldots,l_{|V_1|,1}\rangle\big(H_{G_2}-N_2\mu(G_2)|l_{1,2},\ldots,l_{|V_2|,2}\rangle\big)\ldots|l_{1,k},\ldots,l_{|V_k|,k}\rangle+\cdots\\
&\qquad+|l_{1,1},\ldots,l_{|V_1|,1}\rangle|l_{1,2},\ldots,l_{|V_2|,2}\rangle\ldots\big(H_{G_k}-N_k\mu(G_k)|l_{1,k},\ldots,l_{|V_k|,k}\rangle\big),
\end{aligned}$$

where we used the fact that $\mu(G_i)=\mu(G)$ for $i\in[k]$. From this equation we see that the eigenstates of H_G can be obtained as product states with k factors in the basis (7.10). In each such product state, the ith factor is an eigenstate of $H_{G_i}-N_i\mu(G_i)=H_{G_i}-N_i\mu(G)$ in the N_i-particle sector, with eigenvalue $\lambda_{N_i}^{j_i}(G_i)$. Rewriting this result in the "first-quantized" language, we obtain the Lemma. $\square$

7.1.2.2 QMA-hard problem

With all of these definitions floating around, it will then be useful to actually define the basic problem that we will show is QMA-hard. In particular, we have that for any positive integer α, the following problem:

Problem 3 (α-frustration-free$\mathcal{U}$-interaction MPQW Hamiltonian)**.** We are given as input a K-vertex simple graph G, a number of particles $N \leq K$, and a precision parameter $\epsilon = 1/T$, where the positive integers N and $T \geq 4K$ are given in unary, and the graph G is given as its adjacency matrix (a $K \times K$ symmetric 0-1 matrix). We arp promised that either $\lambda_N^1(G) \leq \epsilon^\alpha$ (a yes instance), or else that $\lambda_N^1(G) \geq \epsilon + \epsilon^\alpha$ (a no instance) and we are asked to decide which is the case.

Note that for each interaction type, this is an infinite family of problems. The positive integer α parameterizes how much the yes cases can deviate from a true frustration-free case. The reason that we define the problem in such a way is that it will facilitate the reduction found in Chapter 8.

Note that this is a special case of the $\mathcal{U}$-interaction MPQW Hamiltonian, with $c = N\mu(G) + \epsilon^\alpha$. As such, if we show that the α-frustration free $\mathcal{U}$-interaction MPQW Hamiltonian problem is QMA-hard, we will also show that the non-frustration-free problem is QMA-complete.

7.2 Constructing the underlying graph for QMA-hardness

At this point, we will want to explicitly construct the graph for which our QMA-hardness result will hold. As such, we will at this point restrict our attention to a particular interaction, $\mathcal{U}$. While the basic idea behind these graphs will not change, the exact graph will depend on both the smallest distance that the interactions occur, as well as the largest distance. We will want to construct a foundational graph that does not have a two-particle ground state, and also we will want to ensure that our connections between these building blocks will not have multiple particles interacting except on specially chosen building blocks.

As such, let us assume that the minimum distance that the interaction $\mathcal{U}$ has non-zero interactions is $d_{\min}$, while the maximum distance is $d_{\max}$. Our graph will only depend on these two quantities.

Additionally, we will want the eventual graph to be a simple graph, so that there is always at most a single edge between two vertices and no self-loops. Unfortunately, our proof strategy will involve adding many positive semi-definite terms to the adjacency matrix, which correspond to adding in edges and self-loops. As such, we will instead force every vertex in the graph to contain a self-loop, so that by removing all of the self loops we only shift the energy levels by a constant amount. Keep this in mind, as the eventual graph is defined.

7.2.1 Gate graphs

In this subsection we define a class of graphs (*gate graphs*) and a diagrammatic notation for them (*gate diagrams*) that will allow us to construct the overall graph. We will also discuss the MPQW Hamiltonian acting on these graphs, with a particular emphasis on the low-energy states.

Every gate graph is constructed using a specific, finite-sized graph g_0 as a building block. This graph is shown in Figure **??** (for graphs with $d_{\min} <= 3$ and discussed in Section **??**. In Section **??** we define gate graphs and gate diagrams. A gate graph is obtained by adding edges and self-loops (in a prescribed way) to a collection of disjoint copies of g_0.

[**TO DO:** *Rewrite this intro*]

In Section **??** we discuss the ground states of the Bose-Hubbard model on gate graphs. For any gate graph G, the smallest eigenvalue $\mu(G)$ of the adjacency matrix $A(G)$ satisfies $\mu(G) \geq -1 - 3\sqrt{2}$. It is convenient to define the constant

$$e_1 = -1 - 3\sqrt{2}. \tag{7.11}$$

When $\mu(G) = e_1$ we say G is an e_1-gate graph. We focus on the frustration-free states of e_1-gate graphs (recall from Definition **??** that $|\phi\rangle \in \mathcal{Z}_N(G)$ is frustration free iff $H(G, N)|\phi\rangle = 0$). We show that all such states live in a convenient subspace (called $\mathcal{I}(G, N)$) of the N-particle Hilbert space. This subspace has the property that no two (or more) particles ever occupy vertices of the same copy of g_0. The restriction to this subspace makes it easier to analyze the ground space.

In Section **??** we consider a class of subspaces that, like $\mathcal{I}(G, N)$, are defined by a set of constraints on the locations of N particles in an e_1-gate graph G. We state an "Occupancy Constraints Lemma" (proven in Appendix **??**) that relates a subspace of this form to the ground space of the Bose-Hubbard model on a graph derived from G.

7.2.1.1 The graph g_0

The graph g_0 shown in Figure **??** is constructed using the method of Chapter 6, with the single qubit circuit corresponding to a sequence of H and HT gates. The idea is to force the ground state of the resulting graph to correspond to these computations while also spreading the wave-function over most of the vertices. In this way, we can use the ground state to compute these single-particle unitaries while also forcing the graph to only have single-particle frustration free states.

In particular, let $k = \max\{d_{\min} + 1, 4\}$, and then let us look at the single-qubit circuit $\mathcal{C}_0$ with k gates U_j, for $j \in [k]$, where

$$U_1 = HT \qquad U_2 = (HT)^{\dagger}$$

and the rest of the $U_j = H$. We can then use the circuit to graph construction from Chapter 6 to construct a simple graph with the ground space spanned by the history states of this circuit.

In this section we map this circuit to the graph g_0. The mapping we use can be generalized to map an arbitrary quantum circuit with any number of qubits to a graph, but for simplicity we focus here on g_0. In Appendix **??** we discuss the more general mapping and use it to prove that computing (in a certain precise sense specified in the Appendix) the smallest eigenvalue of a sparse, efficiently row-computable symmetric 0-1 matrix is QMA-complete.

[**TO DO:** *fix the g_0 graph*]

Starting with the circuit $\mathcal{C}_0$, we apply the Feynman-Kitaev circuit-to-Hamiltonian mapping [?, ?] (up to a constant term and overall multiplicative factor) to get the Hamiltonian

$$-\sqrt{2}\sum_{t=1}^{8}\Big(U_t^\dagger\otimes|t\rangle\langle t+1|+U_t\otimes|t+1\rangle\langle t|\Big). \tag{7.12}$$

This Hamiltonian acts on the Hilbert space $\mathbb{C}^2\otimes\mathbb{C}^8$, where the second register (the "clock register") has periodic boundary conditions (i.e., we let $|8+1\rangle=|1\rangle$). The ground space of (7.12) is spanned by so-called history states

$$|\phi_z\rangle=\frac{1}{\sqrt{8}}\big(|z\rangle(|1\rangle+|3\rangle+|5\rangle+|7\rangle)+H|z\rangle(|2\rangle+|8\rangle)+HT|z\rangle(|4\rangle+|6\rangle)\big),\quad z\in\{0,1\},$$

that encode the history of the computation where the circuit $\mathcal{C}_0$ is applied to $|z\rangle$. One can easily check that $|\phi_z\rangle$ is an eigenstate of the Hamiltonian with eigenvalue $-2\sqrt{2}$.

Now we modify (7.12) to give a symmetric 0-1 matrix. The trick we use is a variant of one used in references [?, ?] for similar purposes.

The nonzero standard basis matrix elements of (7.12) are integer powers of $\omega=e^{i\frac{\pi}{4}}$. Note that ω is an eigenvalue of the 8×8 shift operator

$$S=\sum_{j=0}^{7}|j+1 \bmod 8\rangle\langle j|$$

with eigenvector

$$|\omega\rangle=\frac{1}{\sqrt{8}}\sum_{j=0}^{7}\omega^{-j}|j\rangle.$$

For each operator $-\sqrt{2}H, -\sqrt{2}HT$, or $-\sqrt{2}(HT)^\dagger$ appearing in equation (7.12), define another operator acting on $\mathbb{C}^2\otimes\mathbb{C}^8$ by replacing nonzero matrix elements with powers of the operator S, namely $\omega^k\mapsto S^k$. Write $B(U)$ for the operator obtained by making this replacement in U, e.g.,

$$-\sqrt{2}HT=\begin{pmatrix}\omega^4 & \omega^5\\ \omega^4 & \omega\end{pmatrix}\mapsto B(HT)=\begin{pmatrix}S^4 & S^5\\ S^4 & S\end{pmatrix}.$$

We adjoin an 8-level ancilla and we make this replacement in equation (7.12). This gives

$$H_{\text{prop}}=\sum_{t=1}^{8}\Big(B(U_t)_{13}^\dagger\otimes|t\rangle\langle t+1|_2+B(U_t)_{13}\otimes|t+1\rangle\langle t|_2\Big), \tag{7.13}$$

a symmetric 0-1 matrix acting on $\mathbb{C}^2\otimes\mathbb{C}^8\otimes\mathbb{C}^8$, where the second register is the clock register and the third register is the ancilla register on which the S operators act (the subscripts indicate which registers are acted upon). It is an insignificant coincidence that the clock and ancilla registers have the same dimension.

Note that H_{prop} commutes with S (acting on the 8-level ancilla) and therefore is block diagonal with eight sectors. In the sector where S has eigenvalue ω, it is identical to the

Hamiltonian we started with, equation (7.12). There is also a sector (where S has eigenvalue ω^*) where the Hamiltonian is the entrywise complex conjugate of the one we started with. We add a term to H_{prop} that assigns an energy penalty to states in any of the other six sectors, ensuring that none of these states lie in the ground space of the resulting operator.

Now we can define the graph g_0. Each vertex in g_0 corresponds to a standard basis vector in the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^8 \otimes \mathbb{C}^8$. We label the vertices (z, t, j) with $z \in \{0, 1\}$ describing the state of the computational qubit, $t \in [8]$ giving the state of the clock, and $j \in \{0, \ldots, 7\}$ describing the state of the ancilla. The adjacency matrix is

$$A(g_0) = H_{\text{prop}} + H_{\text{penalty}}$$

where the penalty term

$$H_{\text{penalty}} = \mathbb{I} \otimes \mathbb{I} \otimes \left(S^3 + S^4 + S^5\right)$$

acts nontrivially on the third register. The graph g_0 is shown in Figure **??**.

Now consider the ground space of $A(g_0)$. Note that H_{prop} and H_{penalty} commute, so they can be simultaneously diagonalized. Furthermore, H_{penalty} has smallest eigenvalue $-1 - \sqrt{2}$ (with eigenspace spanned by $|\omega\rangle$ and $|\omega^*\rangle$) and first excited energy -1. The norm of H_{prop} satisfies $\|H_{\text{prop}}\| \leq 4$, which follows from the fact that H_{prop} has four ones in each row and column (with the remaining entries all zero).

The smallest eigenvalue of $A(g_0)$ lives in the sector where H_{penalty} has eigenvalue $-1-\sqrt{2}$ and is equal to

$$-2\sqrt{2} + (-1 - \sqrt{2}) = -1 - 3\sqrt{2} = -5.24\ldots. \tag{7.14}$$

This is the constant e_1 from equation (7.11). To see this, note that in any other sector H_{penalty} has eigenvalue at least -1 and every eigenvalue of $A(g_0)$ is at least -5 (using the fact that $H_{\text{prop}} \geq -4$). An orthonormal basis for the ground space of $A(g_0)$ is furnished by the states

$$|\psi_{z,0}\rangle = \frac{1}{\sqrt{8}}\big(|z\rangle(|1\rangle + |3\rangle + |5\rangle + |7\rangle) + H|z\rangle(|2\rangle + |8\rangle) + HT|z\rangle(|4\rangle + |6\rangle)\big)|\omega\rangle \tag{7.15}$$

$$|\psi_{z,1}\rangle = |\psi_{z,0}\rangle^* \tag{7.16}$$

where $z \in \{0, 1\}$.

Note that the amplitudes of $|\psi_{z,0}\rangle$ in the above basis contain the result of computing either the identity, Hadamard, or HT gate acting on the "input" state $|z\rangle$.

7.2.1.2 Gate graphs

We use three different schematic representations of the graph g_0 (defined in Section **??**), as depicted in Figure **??**. We call these Figures *diagram elements*; they are also the simplest examples of *gate diagrams*, which we define shortly.

The black and grey circles in a diagram element are called "nodes." Each node has a label (z, t). The only difference between the three diagram elements is the labeling of their nodes. In particular, the nodes in the diagram element $U \in \{\mathbb{I}, H, HT\}$ correspond to values of $t \in [8]$ where the first register in equation (7.15) is either $|z\rangle$ or $U|z\rangle$. For example, the nodes for the H diagram element have labels with $t \in \{1, 3\}$ (where $|\psi_{z,0}\rangle$ contains the "input" $|z\rangle$) or $t = \{2, 8\}$ (where $|\psi_{z,0}\rangle$ contains the "output" $H|z\rangle$). We draw the input nodes in black and the output nodes in grey.

The rules for constructing gate diagrams are simple. A gate diagram consists of some number $R \in \{1, 2, \ldots\}$ of diagram elements, with self-loops attached to a subset $\mathcal{S}$ of the nodes and edges connecting a set $\mathcal{E}$ of pairs of nodes. A node may have a single edge or a single self-loop attached to it, but never more than one edge or self-loop and never both an edge and a self-loop. Each node in a gate diagram has a label (q, z, t) where $q \in [R]$ indicates the diagram element it belongs to. An example is shown in Figure **??**. Sometimes it is convenient to draw the input nodes on the right-hand side of a diagram element; e.g., in Figure **??** the node closest to the top left corner is labeled $(q, z, t) = (3, 0, 2)$.

To every gate diagram we associate a *gate graph* G with vertex set

$$\{(q, z, t, j) \colon q \in [R],\ z \in \{0, 1\},\ t \in [8],\ j \in \{0, \ldots, 7\}\}$$

and adjacency matrix

$$A(G) = \mathbb{I}_q \otimes A(g_0) + h_{\mathcal{S}} + h_{\mathcal{E}} \tag{7.17}$$

$$h_{\mathcal{S}} = \sum_{\mathcal{S}} |q, z, t\rangle\langle q, z, t| \otimes \mathbb{I}_j \tag{7.18}$$

$$h_{\mathcal{E}} = \sum_{\mathcal{E}} \left(|q, z, t\rangle + |q', z', t'\rangle\right)\left(\langle q, z, t| + \langle q', z', t'|\right) \otimes \mathbb{I}_j. \tag{7.19}$$

The sums in equations (7.18) and (7.19) run over the set of nodes with self-loops $(q, z, t) \in \mathcal{S}$ and the set of pairs of nodes connected by edges $\{(q, z, t), (q', z', t')\} \in \mathcal{E}$, respectively. We write $\mathbb{I}_q$ and $\mathbb{I}_j$ for the identity operator on the registers with variables q and j, respectively. We see from the above expression that each self-loop in the gate diagram corresponds to 8 self-loops in the graph G, and an edge in the gate diagram corresponds to 8 edges and 16 self-loops in G.

Since a node in a gate graph never has more than one edge or self-loop attached to it, equations (7.18) and (7.19) are sums of orthogonal Hermitian operators. Therefore

$$\|h_{\mathcal{S}}\| = \max_{\mathcal{S}} \||q, z, t\rangle\langle q, z, t| \otimes \mathbb{I}_j\| = 1 \quad \text{if } \mathcal{S} \neq \emptyset \tag{7.20}$$

$$\|h_{\mathcal{E}}\| = \max_{\mathcal{E}} \|\left(|q, z, t\rangle + |q', z', t'\rangle\right)\left(\langle q, z, t| + \langle q', z', t'|\right) \otimes \mathbb{I}_j\| = 2 \quad \text{if } \mathcal{E} \neq \emptyset \tag{7.21}$$

for any gate graph. (Of course, this also shows that $\|h_{\mathcal{S}'}\| = 1$ and $\|h_{\mathcal{E}'}\| = 2$ for any nonempty subsets $\mathcal{S}' \subseteq \mathcal{S}$ and $\mathcal{E}' \subseteq \mathcal{E}$.)

[**TO DO:** *Change this to the updated types with every vertex having a self-loop*]

7.2.1.3 Frustration-free states for a given interaction range

Consider the adjacency matrix $A(G)$ of a gate graph G, and note (from equation (7.17) that its smallest eigenvalue $\mu(G)$ satisfies

$$\mu(G) \geq e_1$$

since $h_{\mathcal{S}}$ and $h_{\mathcal{E}}$ are positive semidefinite and $A(g_0)$ has smallest eigenvalue e_1. In the special case where $\mu(G) = e_1$, we say G is an e_1-gate graph.

Definition 7. An e_1-gate graph is a gate graph G such that the smallest eigenvalue of its adjacency matrix is $e_1 = -1 - 3\sqrt{2}$.

When G is an e_1-gate graph, a single-particle ground state $|\Gamma\rangle$ of $A(G)$ satisfies

$$(\mathbb{I} \otimes A(g_0))\,|\Gamma\rangle = e_1|\Gamma\rangle \tag{7.22}$$
$$h_{\mathcal{S}}|\Gamma\rangle = 0 \tag{7.23}$$
$$h_{\mathcal{E}}|\Gamma\rangle = 0. \tag{7.24}$$

Indeed, to show that a given gate graph G is an e_1-gate graph, it suffices to find a state $|\Gamma\rangle$ satisfying these conditions. Note that equation (7.22) implies that $|\Gamma\rangle$ can be written as a superposition of the states

$$|\psi^q_{z,a}\rangle = |q\rangle|\psi_{z,a}\rangle, \quad z, a \in \{0,1\},\, q \in [R]$$

where $|\psi_{z,a}\rangle$ is given by equations (7.15) and (7.16). The coefficients in the superposition are then constrained by equations (7.23) and (7.24).

Example 1. As an example, we show the gate graph in Figure **??** is an e_1-gate graph. As noted above, equation (7.22) lets us restrict our attention to the space spanned by the eight states $|\psi^q_{z,a}\rangle$ with $z, a \in \{0,1\}$ and $q \in \{1,2\}$. In this basis, the operators $h_{\mathcal{S}}$ and $h_{\mathcal{E}}$ only have nonzero matrix elements between states with the same value of $a \in \{0,1\}$. We therefore solve for the e_1 energy ground states with $a = 0$ and those with $a = 1$ separately. Consider a ground state of the form

$$\left(\tau_1|\psi^1_{0,a}\rangle + \nu_1|\psi^1_{1,a}\rangle\right) + \left(\tau_2|\psi^2_{0,a}\rangle + \nu_2|\psi^2_{1,a}\rangle\right)$$

and note that in this case (7.23) implies $\tau_1 = 0$. Equation (7.24) gives

$$\begin{pmatrix}\tau_2\\ \nu_2\end{pmatrix} = \begin{cases} HT\begin{pmatrix}-\tau_1\\ -\nu_1\end{pmatrix} & a = 0\\ (HT)^*\begin{pmatrix}-\tau_1\\ -\nu_1\end{pmatrix} & a = 1.\end{cases}$$

We find two orthogonal e_1-energy states, which are (up to normalization)

$$|\psi^1_{1,0}\rangle - \frac{e^{i\frac{\pi}{4}}}{\sqrt{2}}\left(|\psi^2_{0,0}\rangle - |\psi^2_{1,0}\rangle\right) \tag{7.25}$$
$$|\psi^1_{1,1}\rangle - \frac{e^{-i\frac{\pi}{4}}}{\sqrt{2}}\left(|\psi^2_{0,1}\rangle - |\psi^2_{1,1}\rangle\right). \tag{7.26}$$

We interpret each of these states as encoding a qubit that is transformed at each set of input/output nodes in the gate diagram in Figure **??**. The encoded qubit begins on the input nodes of the first diagram element in the state

$$\begin{pmatrix}\tau_1\\ \nu_1\end{pmatrix} = \begin{pmatrix}0\\ 1\end{pmatrix}$$

because the self-loop penalizes the basis vectors $|\psi^1_{0,a}\rangle$. On the output nodes of diagram element 1, the encoded qubit is in the state where either HT (if $a = 0$) or its complex conjugate (if $a = 1$) has been applied. The edges in the gate diagram ensure that the encoded qubit on the input nodes of diagram element 2 is minus the state on the output nodes of diagram element 1.

In this example, each single-particle ground state encodes a single-qubit computation. Later we show how N-particle frustration-free states on e_1-gate graphs can encode computations on N qubits. Recall from Definition **??** that a state $|\Gamma\rangle \in \mathcal{Z}_N(G)$ is said to be frustration free iff $H(G,N)|\Gamma\rangle = 0$. Note that $H(G,N) \geq 0$, so an N-particle frustration-free state is necessarily a ground state. Putting this together with Lemma **??**, we see that the existence of an N-particle frustration-free state implies

$$\lambda^1_N(G) = \lambda^1_{N-1}(G) = \ldots = \lambda^1_1(G) = 0,$$

i.e., there are N'-particle frustration-free states for all $N' \leq N$.

We prove that the graph g_0 has no two-particle frustration-free states. By Lemma **??**, it follows that g_0 has no N-particle frustration-free states for $N \geq 2$.

Lemma 13. $\lambda^1_2(g_0) > 0$.

Proof. Suppose (for a contradiction) that $|Q\rangle \in \mathcal{Z}_2(g_0)$ is a nonzero vector in the nullspace of $H(g_0, 2)$, so

$$H^2_{g_0}|Q\rangle = \left(A(g_0) \otimes \mathbb{I} + \mathbb{I} \otimes A(g_0) + 2\sum_{v\in g_0} |v\rangle\langle v| \otimes |v\rangle\langle v|\right)|Q\rangle = 2e_1|Q\rangle.$$

This implies

$$A(g_0) \otimes \mathbb{I}|Q\rangle = \mathbb{I} \otimes A(g_0)|Q\rangle = e_1|Q\rangle$$

since $A(g_0)$ has smallest eigenvalue e_1 and the interaction term is positive semidefinite. We can therefore write

$$|Q\rangle = \sum_{z,a,x,y\in\{0,1\}} Q_{za,xy}|\psi_{z,a}\rangle|\psi_{x,y}\rangle$$

with $Q_{za,xy} = Q_{xy,za}$ (since $|Q\rangle \in \mathcal{Z}_2(g_0)$) and

$$\left(|v\rangle\langle v| \otimes |v\rangle\langle v|\right)|Q\rangle = 0 \tag{7.27}$$

for all vertices $v = (z,t,j) \in g_0$. Using this equation with $|v\rangle = |0,1,j\rangle$ gives

$$\begin{aligned}
&Q_{00,00}\langle 0,1,j|\psi_{0,0}\rangle^2 + 2Q_{01,00}\langle 0,1,j|\psi_{0,1}\rangle\langle 0,1,j|\psi_{0,0}\rangle + Q_{01,01}\langle 0,1,j|\psi_{0,1}\rangle^2 \\
&\quad = \frac{1}{64}\left(Q_{00,00}i^{-j} + 2Q_{01,00} + Q_{01,01}i^j\right) \\
&\quad = 0
\end{aligned}$$

for each $j \in \{0, \ldots, 7\}$. The only solution to this set of equations is $Q_{00,00} = Q_{01,00} = Q_{01,01} = 0$. The same analysis, now using $|v\rangle = |1, 1, j\rangle$, gives $Q_{10,10} = Q_{11,10} = Q_{11,11} = 0$. Finally, using equation (7.27) with $|v\rangle = |0, 2, j\rangle$ gives

$$\begin{aligned}
&\frac{1}{64}\langle 0|H|1\rangle\langle 0|H|0\rangle \left(2Q_{10,00}i^{-j} + 2Q_{10,01} + 2Q_{11,00} + 2Q_{11,01}i^{j}\right) \\
&\quad = \frac{1}{64}\left(Q_{10,00}i^{-j} + Q_{10,01} + Q_{11,00} + Q_{11,01}i^{j}\right) \\
&\quad = 0
\end{aligned}$$

for all $j \in \{0, \ldots, 7\}$, which implies that $Q_{10,00} = Q_{11,01} = 0$ and $Q_{11,00} = -Q_{10,01}$. Thus, up to normalization,

$$|Q\rangle = |\psi_{1,0}\rangle|\psi_{0,1}\rangle + |\psi_{0,1}\rangle|\psi_{1,0}\rangle - |\psi_{11}\rangle|\psi_{00}\rangle - |\psi_{00}\rangle|\psi_{11}\rangle.$$

Now applying equation (7.27) with $|v\rangle = |0, 4, j\rangle$, we see that the quantity

$$\frac{1}{64}\left(2\langle 0|HT|1\rangle\langle 0|(HT)^{*}|0\rangle - 2\langle 0|(HT)^{*}|1\rangle\langle 0|HT|0\rangle\right) = \frac{1}{64}\left(e^{i\frac{\pi}{4}} - e^{-i\frac{\pi}{4}}\right)$$

must be zero, which is a contradiction. Hence we conclude that the nullspace of $H(g_0, 2)$ is empty. □

We now characterize the space of N-particle frustration-free states on an e_1-gate graph G. Define the subspace $\mathcal{I}(G, N) \subset \mathcal{Z}_N(G)$ where each particle is in a ground state of $A(g_0)$ and no two particles are located within the same diagram element:

$$\mathcal{I}(G, N) = \operatorname{span}\{\operatorname{Sym}(|\psi^{q_1}_{z_1,a_1}\rangle \ldots |\psi^{q_N}_{z_N,a_N}\rangle)\colon z_i, a_i \in \{0, 1\},\ q_i \in [R],\ q_i \neq q_j \text{ whenever } i \neq j\}. \tag{7.28}$$

Lemma 14. *Let G be an e_1-gate graph. A state $|\Gamma\rangle \in \mathcal{Z}_N(G)$ is frustration free if and only if*

$$(A(G) - e_1)^{(w)}|\Gamma\rangle = 0 \quad \textit{for all } w \in [N] \tag{7.29}$$

$$|\Gamma\rangle \in \mathcal{I}(G, N). \tag{7.30}$$

Proof. First suppose that equations (7.29) and (7.30) hold. From (7.30) we see that $|\Gamma\rangle$ has no support on states where two or more particles are located at the same vertex. Hence

$$\sum_{k \in V} \hat{n}_k\left(\hat{n}_k - 1\right)|\Gamma\rangle = 0. \tag{7.31}$$

Putting together equations (7.29) and (7.31), we get

$$H(G, N)|\Gamma\rangle = \left(H^N_G - Ne_1\right)|\Gamma\rangle = 0,$$

so $|\Gamma\rangle$ is frustration free.

To complete the proof, we show that if $|\Gamma\rangle$ is frustration free, then conditions (7.29) and (7.30) hold. By definition, a frustration-free state $|\Gamma\rangle$ satisfies

$$H(G,N)|\Gamma\rangle = \left(\sum_{w=1}^{N} \left(A(G)-e_1\right)^{(w)} + \sum_{k\in V} \hat{n}_k\left(\hat{n}_k - 1\right)\right)|\Gamma\rangle = 0. \qquad (7.32)$$

Since both terms in the large parentheses are positive semidefinite, they must both annihilate $|\Gamma\rangle$ (similarly, each term in the first summation must be zero). Hence equation (7.29) holds. Let G_{rem} be the graph obtained from G by removing all of the edges and self-loops in the gate diagram of G. In other words,

$$A(G_{\text{rem}}) = \sum_{q=1}^{R} |q\rangle\langle q| \otimes A(g_0) = \mathbb{I}\otimes A(g_0).$$

Noting that

$$H(G,N) \geq H(G_{\text{rem}},N) \geq 0,$$

we see that equation (7.32) also implies

$$H(G_{\text{rem}},N)|\Gamma\rangle = 0. \qquad (7.33)$$

Since each of the R components of G_{rem} is an identical copy of g_0, the eigenvalues and eigenvectors of $H(G_{\text{rem}},N)$ are characterized by Lemma 12 (along with knowledge of the eigenvalues and eigenvectors of g_0). By Lemma 13 and Lemma **??**, no component has a two- (or more) particle frustration-free state. Combining these two facts, we see that in an N-particle frustration-free state, every component of G_{rem} must contain either 0 or 1 particles, and the nullspace of $H(G_{\text{rem}},N)$ is the space $\mathcal{I}(G,N)$. From equation (7.33) we get $|\Gamma\rangle \in \mathcal{I}(G,N)$. □

Note that if $\mathcal{I}(G,N)$ is empty then Lemma 14 says that G has no N-particle frustration-free states. For example, this holds for any e_1-gate graph G whose gate diagram has $R < N$ diagram elements.

A useful consequence of Lemma 14 is the fact that every k-particle reduced density matrix of an N-particle frustration-free state $|\Gamma\rangle$ on an e_1-gate graph G (with $k \leq N$) has all of its support on k-particle frustration-free states. To see this, note that for any partition of the N registers into subsets A (of size k) and B (of size $N-k$), we have

$$\mathcal{I}(G,N) \subseteq \mathcal{I}(G,k)_A \otimes \mathcal{Z}_{N-k}(G)_B.$$

Thus, if condition (7.30) holds, then all k-particle reduced density matrices of $|\Gamma\rangle$ are contained in $\mathcal{I}(G,k)$. Furthermore, (7.29) is a statement about the single-particle reduced density matrices, so it also holds for each k-particle reduced density matrix. From this we see that each reduced density matrix of $|\Gamma\rangle$ is frustration free.

7.2.2 Gadgets

In Example 1 we saw how a single-particle ground state can encode a single-qubit computation. In this Section we see how a two-particle frustration-free state on a suitably designed e_1-gate graph can encode a two-qubit computation. We design specific e_1-gate graphs (called *gadgets*) that we use in Section **??** to prove that Bose-Hubbard Hamiltonian is QMA-hard. For each gate graph we discuss, we show that the smallest eigenvalue of its adjacency matrix is e_1 and we solve for all of the frustration-free states.

We first design a gate graph where, in any two-particle frustration-free state, the locations of the particles are synchronized. This "move-together" gadget is presented in Section **??**. In Section **??**, we design gadgets for two-qubit gates using four move-together gadgets, one for each two-qubit computational basis state. Finally, in Section **??** we describe a small modification of a two-qubit gate gadget called the "boundary gadget."

The circuit-to-gate graph mapping described in Section **??** uses a two-qubit gate gadget for each gate in the circuit, together with boundary gadgets in parts of the graph corresponding to the beginning and end of the computation.

The gate diagram for the *move-together gadget* is shown in Figure **??**. Using equation (7.17), we write the adjacency matrix of the corresponding gate graph G_W as

$$A(G_W) = \sum_{q=1}^{6} |q\rangle\langle q| \otimes A(g_0) + h_{\mathcal{E}} \tag{7.34}$$

where $h_{\mathcal{E}}$ is given by (7.19) and $\mathcal{E}$ is the set of edges in the gate diagram (in this case $h_{\mathcal{S}} = 0$ as there are no self-loops).

We begin by solving for the single-particle ground states, i.e., the eigenvectors of (7.34) with eigenvalue $e_1 = -1 - 3\sqrt{2}$. As in Example 1, we can solve for the states with $a = 0$ and $a = 1$ separately, since

$$\langle \psi^j_{x,1} | h_{\mathcal{E}} | \psi^i_{z,0} \rangle = 0$$

for all $i, j \in \{1, \ldots, 6\}$ and $x, z \in \{0, 1\}$. We write a single-particle ground state as

$$\sum_{i=1}^{6} \left(\tau_i |\psi^i_{0,a}\rangle + \nu_i |\psi^i_{1,a}\rangle \right)$$

and solve for the coefficients τ_i and ν_i using equation (7.24) (in this case equation (7.23) is automatically satisfied since $h_{\mathcal{S}} = 0$). Enforcing (7.24) gives eight equations, one for each edge in the gate diagram:

$$\begin{aligned}
\tau_3 &= -\tau_1 & \qquad \frac{1}{\sqrt{2}}(\tau_1 + \nu_1) &= -\tau_6 \\
\tau_4 &= -\nu_1 & \frac{1}{\sqrt{2}}(\tau_1 - \nu_1) &= -\tau_5 \\
\nu_3 &= -\tau_2 & \frac{1}{\sqrt{2}}(\tau_2 + \nu_2) &= -\nu_5 \\
\nu_4 &= -\nu_2 & \frac{1}{\sqrt{2}}(\tau_2 - \nu_2) &= -\nu_6.
\end{aligned}$$

There are four linearly independent solutions to this set of equations, given by

$$\begin{array}{llllll}
\textit{Solution 1:} & \tau_1 = 1 & \tau_3 = -1 & \tau_5 = -\frac{1}{\sqrt{2}} & \tau_6 = -\frac{1}{\sqrt{2}} & \text{all other coefficients 0} \\
\textit{Solution 2:} & \nu_1 = 1 & \tau_4 = -1 & \tau_5 = \frac{1}{\sqrt{2}} & \tau_6 = -\frac{1}{\sqrt{2}} & \text{all other coefficients 0} \\
\textit{Solution 3:} & \nu_2 = 1 & \nu_4 = -1 & \nu_5 = -\frac{1}{\sqrt{2}} & \nu_6 = \frac{1}{\sqrt{2}} & \text{all other coefficients 0} \\
\textit{Solution 4:} & \tau_2 = 1 & \nu_3 = -1 & \nu_5 = -\frac{1}{\sqrt{2}} & \nu_6 = -\frac{1}{\sqrt{2}} & \text{all other coefficients 0.}
\end{array}$$

For each of these solutions, and for each $a \in \{0,1\}$, we find a single-particle state with energy e_1. This result is summarized in the following Lemma.

Lemma 15. *G_W is an e_1-gate graph. A basis for the eigenspace of $A(G_W)$ with eigenvalue e_1 is*

$$|\chi_{1,a}\rangle = \frac{1}{\sqrt{3}}|\psi^1_{0,a}\rangle - \frac{1}{\sqrt{3}}|\psi^3_{0,a}\rangle - \frac{1}{\sqrt{6}}|\psi^5_{0,a}\rangle - \frac{1}{\sqrt{6}}|\psi^6_{0,a}\rangle \tag{7.35}$$

$$|\chi_{2,a}\rangle = \frac{1}{\sqrt{3}}|\psi^1_{1,a}\rangle - \frac{1}{\sqrt{3}}|\psi^4_{0,a}\rangle + \frac{1}{\sqrt{6}}|\psi^5_{0,a}\rangle - \frac{1}{\sqrt{6}}|\psi^6_{0,a}\rangle \tag{7.36}$$

$$|\chi_{3,a}\rangle = \frac{1}{\sqrt{3}}|\psi^2_{1,a}\rangle - \frac{1}{\sqrt{3}}|\psi^4_{1,a}\rangle - \frac{1}{\sqrt{6}}|\psi^5_{1,a}\rangle + \frac{1}{\sqrt{6}}|\psi^6_{1,a}\rangle \tag{7.37}$$

$$|\chi_{4,a}\rangle = \frac{1}{\sqrt{3}}|\psi^2_{0,a}\rangle - \frac{1}{\sqrt{3}}|\psi^3_{1,a}\rangle - \frac{1}{\sqrt{6}}|\psi^5_{1,a}\rangle - \frac{1}{\sqrt{6}}|\psi^6_{1,a}\rangle \tag{7.38}$$

where $a \in \{0,1\}$.

In Figure **??** we have used a shorthand $\alpha, \beta, \gamma, \delta$ to identify four nodes of the move-together gadget; these are the nodes with labels $(q,z,t) = (1,0,1), (1,1,1), (2,1,1), (2,0,1)$, respectively. We view α and γ as "input" nodes and β and δ as "output" nodes for this gate diagram. It is natural to associate each single-particle state $|\chi_{i,a}\rangle$ with one of these four nodes. We also associate the set of 8 vertices represented by the node with the corresponding node, e.g.,

$$S_\alpha = \{(1,0,1,j) \colon j \in \{0,\ldots,7\}\}.$$

Looking at equation (7.35) (and perhaps referring back to equation (7.15)) we see that $|\chi_{1,a}\rangle$ has support on vertices in S_α but not on vertices in S_β, S_γ, or S_δ. Looking at the picture on the right-hand side of the equality sign in Figure **??**, we think of $|\chi_{1,a}\rangle$ as localized at the node α, with no support on the other three nodes. The states $|\chi_{2,a}\rangle, |\chi_{3,a}\rangle, |\chi_{4,a}\rangle$ are similarly localized at nodes β, γ, δ. We view $|\chi_{1,a}\rangle$ and $|\chi_{3,a}\rangle$ as input states and $|\chi_{2,a}\rangle$ and $|\chi_{4,a}\rangle$ as output states.

Now we turn our attention to the two-particle frustration-free states of the move-together gadget, i.e., the states $|\Phi\rangle \in \mathcal{Z}_2(G_W)$ in the nullspace of $H(G_W, 2)$. Using Lemma 14 we can write

$$|\Phi\rangle = \sum_{a,b\in\{0,1\},\, I,J\in[4]} C_{(I,a),(J,b)}|\chi_{I,a}\rangle|\chi_{J,b}\rangle \tag{7.39}$$

where the coefficients are symmetric, i.e.,

$$C_{(I,a),(J,b)} = C_{(J,b),(I,a)}, \tag{7.40}$$

and where

$$\langle \psi^q_{z,a} | \langle \psi^q_{x,b} | \Phi \rangle = 0 \tag{7.41}$$

for all $z, a, x, b \in \{0, 1\}$ and $q \in [6]$.

The move-together gadget is designed so that each solution $|\Phi\rangle$ to these equations is a superposition of a term where both particles are in input states and a term where both particles are in output states. The particles move from input nodes to output nodes together. We now solve equations (7.39)–(7.41) and prove the following.

Lemma 16. *A basis for the nullspace of $H(G_W, 2)$ is*

$$|\Phi_{a,b}\rangle = \mathrm{Sym}\left(\frac{1}{\sqrt{2}}|\chi_{1,a}\rangle|\chi_{3,b}\rangle + \frac{1}{\sqrt{2}}|\chi_{2,a}\rangle|\chi_{4,b}\rangle\right), \quad a, b \in \{0, 1\}. \tag{7.42}$$

There are no N-particle frustration-free states on G_W for $N \geq 3$, i.e.,

$$\lambda^1_N(G_W) > 0 \quad \textit{for } N \geq 3.$$

Proof. The states $|\Phi_{a,b}\rangle$ manifestly satisfy equations (7.39) and (7.40), and one can directly verify that they also satisfy (7.41) (the nontrivial cases to check are $q = 5$ and $q = 6$).

To complete the proof that (7.42) is a basis for the nullspace of $H(G_W, 2)$, we verify that any state satisfying these conditions must be a linear combination of these four states. Applying equation (7.41) gives

$$\begin{aligned}
\langle \psi^1_{0,a} | \langle \psi^1_{0,b} | \Phi \rangle &= \frac{1}{3} C_{(1,a),(1,b)} = 0 & \qquad \langle \psi^1_{1,a} | \langle \psi^1_{1,b} | \Phi \rangle &= \frac{1}{3} C_{(2,a),(2,b)} = 0 \\
\langle \psi^2_{1,a} | \langle \psi^2_{1,b} | \Phi \rangle &= \frac{1}{3} C_{(3,a),(3,b)} = 0 & \qquad \langle \psi^2_{0,a} | \langle \psi^2_{0,b} | \Phi \rangle &= \frac{1}{3} C_{(4,a),(4,b)} = 0 \\
\langle \psi^1_{0,a} | \langle \psi^1_{1,b} | \Phi \rangle &= \frac{1}{3} C_{(1,a),(2,b)} = 0 & \qquad \langle \psi^2_{0,a} | \langle \psi^2_{1,b} | \Phi \rangle &= \frac{1}{3} C_{(4,a),(3,b)} = 0 \\
\langle \psi^3_{0,a} | \langle \psi^3_{1,b} | \Phi \rangle &= \frac{1}{3} C_{(1,a),(4,b)} = 0 & \qquad \langle \psi^4_{0,a} | \langle \psi^4_{1,b} | \Phi \rangle &= \frac{1}{3} C_{(2,a),(3,b)} = 0
\end{aligned}$$

for all $a, b \in \{0, 1\}$. Using the fact that all of these coefficients are zero, and using equation (7.40), we get

$$|\Phi\rangle = \sum_{a,b \in \{0,1\}} \left(C_{(1,a),(3,b)} \left(|\chi_{1,a}\rangle|\chi_{3,b}\rangle + |\chi_{3,b}\rangle|\chi_{1,a}\rangle \right) + C_{(2,a),(4,b)} \left(|\chi_{2,a}\rangle|\chi_{4,b}\rangle + |\chi_{4,b}\rangle|\chi_{2,a}\rangle \right) \right).$$

Finally, applying equation (7.41) again gives

$$\langle \psi^6_{0,a} | \langle \psi^6_{1,b} | \Phi \rangle = \frac{1}{6} C_{(2,a),(4,b)} - \frac{1}{6} C_{(1,a),(3,b)} = 0.$$

Hence

$$|\Phi\rangle = \sum_{a,b \in \{0,1\}} C_{(1,a),(3,b)} \left(|\chi_{1,a}\rangle|\chi_{3,b}\rangle + |\chi_{3,b}\rangle|\chi_{1,a}\rangle + |\chi_{2,a}\rangle|\chi_{4,b}\rangle + |\chi_{4,b}\rangle|\chi_{2,a}\rangle \right),$$

which is a superposition of the states $|\Phi_{a,b}\rangle$.

Finally, we prove that there are no frustration-free ground states of the Bose-Hubbard model on G_W with more than two particles. By Lemma **??**, it suffices to prove that there are no frustration-free three-particle states.

Suppose (for a contradiction) that $|\Gamma\rangle \in \mathcal{Z}_3(G_W)$ is a normalized three-particle frustration-free state. Write

$$|\Gamma\rangle = \sum D_{(i,a),(j,b),(k,c)}|\chi_{i,a}\rangle|\chi_{j,b}\rangle|\chi_{k,c}\rangle.$$

Note that each reduced density matrix of $|\Gamma\rangle$ on two of the three subsystems must have all of its support on two-particle frustration-free states (see the remark following Lemma 14), i.e., on the states $|\Phi_{a,b}\rangle$. Using this fact for the subsystem consisting of the first two particles, we see in particular that

$$(i,j) \notin \{(1,3),(3,1),(2,4),(4,2)\} \quad \Longrightarrow \quad D_{(i,a),(j,b),(k,c)} = 0 \tag{7.43}$$

(since $|\Phi_{a_1,a_2}\rangle$ only has support on vectors $|\chi_{i,a}\rangle|\chi_{j,b}\rangle$ with $i,j \in \{(1,3),(3,1),(2,4),(4,2)\}$).

Using this fact for subsystems consisting of particles $2,3$ and $1,3$, respectively, gives

$$(j,k) \notin \{(1,3),(3,1),(2,4),(4,2)\} \quad \Longrightarrow \quad D_{(i,a),(j,b),(k,c)} = 0 \tag{7.44}$$

$$(i,k) \notin \{(1,3),(3,1),(2,4),(4,2)\} \quad \Longrightarrow \quad D_{(i,a),(j,b),(k,c)} = 0. \tag{7.45}$$

Putting together equations (7.43), (7.44), and (7.45), we see that $|\Gamma\rangle = 0$. This is a contradiction, so no three-particle frustration-free states exist. $\square$

Next we show how this gadget can be used to build gadgets the implement two-qubit gates.

7.2.2.1 Two-qubit gate gadget

In this Section we define a gate graph for each of the two-qubit unitaries

$$\{\mathrm{CNOT}_{12}, \mathrm{CNOT}_{21}, \mathrm{CNOT}_{12}\left(H \otimes \mathbb{I}\right), \mathrm{CNOT}_{12}\left(HT \otimes \mathbb{I}\right)\}.$$

Here CNOT_{12} is the standard controlled-not gate with the second qubit as a target, whereas CNOT_{21} has the first qubit as target.

We define the gate graphs by exhibiting their gate diagrams. For the three cases

$$U = \mathrm{CNOT}_{12}(\tilde{U} \otimes \mathbb{I})$$

with $\tilde{U} \in \{\mathbb{I}, H, HT\}$, we associate U with the gate diagram shown in Figure **??**. In the Figure we also indicate a shorthand used to represent this gate diagram. As one might expect, for the case $U = \mathrm{CNOT}_{21}$, we use the same gate diagram as for $U = \mathrm{CNOT}_{12}$; however, we use the slightly different shorthand shown in Figure **??**.

Roughly speaking, the two-qubit gate gadgets work as follows. In Figure **??** there are four move-together gadgets, one for each two-qubit basis state $|00\rangle, |01\rangle, |10\rangle, |11\rangle$. These enforce the constraint that two particles must move through the graph together. The connections between the four diagram elements labeled $1,2,3,4$ and the move-together gadgets ensure that certain frustration-free two-particle states encode two-qubit computations, while the connections between diagram elements $1, 2, 3, 4$ and $5, 6, 7, 8$ ensure that there are no additional frustration-free two-particle states (i.e., states that do not encode computations).

To describe the frustration-free states of the gate graph depicted in Figure **??**, first recall the definition of the states $|\chi_{1,a}\rangle, |\chi_{2,a}\rangle, |\chi_{3,a}\rangle, |\chi_{4,a}\rangle$ from equations (7.35)–(7.38). For each of the move-together gadgets $xy \in \{00, 01, 10, 11\}$ in Figure **??**, write

$$|\chi^{xy}_{L,a}\rangle$$

for the state $|\chi_{L,a}\rangle$ with support (only) on the gadget labeled xy. Write

$$U(a) = \begin{cases} U & \text{if } a = 0 \\ U^* & \text{if } a = 1 \end{cases}$$

and similarly for $\tilde{U}$ (we use this notation throughout the paper to indicate a unitary or its elementwise complex conjugate).

In Appendix **??** we prove the following Lemma, which shows that G_U is an e_1-gate graph and solves for its frustration-free states.

Lemma 17. *Let $U = \mathrm{CNOT}_{12}(\tilde{U} \otimes \mathbb{I})$ where $\tilde{U} \in \{\mathbb{I}, H, HT\}$. The corresponding gate graph G_U is defined by its gate diagram shown in Figure **??**. The adjacency matrix $A(G_U)$ has ground energy e_1; a basis for the corresponding eigenspace is*

$$|\rho^{1,U}_{z,a}\rangle = \frac{1}{\sqrt{8}}|\psi^1_{z,a}\rangle - \frac{1}{\sqrt{8}}|\psi^{5+z}_{z,a}\rangle - \sqrt{\frac{3}{8}}\sum_{x,y=0}^{1}\tilde{U}(a)_{yz}|\chi^{yx}_{1,a}\rangle \quad |\rho^{2,U}_{z,a}\rangle = \frac{1}{\sqrt{8}}|\psi^2_{z,a}\rangle - \frac{1}{\sqrt{8}}|\psi^{6-z}_{z,a}\rangle - \sqrt{\frac{3}{8}}\sum_{x=0}^{1}|\chi^{zx}_{2,a}\rangle \tag{7.46}$$

$$|\rho^{3,U}_{z,a}\rangle = \frac{1}{\sqrt{8}}|\psi^3_{z,a}\rangle - \frac{1}{\sqrt{8}}|\psi^{7}_{z,a}\rangle - \sqrt{\frac{3}{8}}\sum_{x=0}^{1}|\chi^{xz}_{3,a}\rangle \quad |\rho^{4,U}_{z,a}\rangle = \frac{1}{\sqrt{8}}|\psi^4_{z,a}\rangle - \frac{1}{\sqrt{8}}|\psi^{8}_{z,a}\rangle - \sqrt{\frac{3}{8}}\sum_{x=0}^{1}|\chi^{x(z\oplus x)}_{4,a}\rangle \tag{7.47}$$

where $z, a \in \{0, 1\}$. A basis for the nullspace of $H(G_U, 2)$ is

$$\mathrm{Sym}(|T^U_{z_1,a,z_2,b}\rangle), \quad z_1, z_2, a, b \in \{0, 1\} \tag{7.48}$$

where

$$|T^U_{z_1,a,z_2,b}\rangle = \frac{1}{\sqrt{2}}|\rho^{1,U}_{z_1,a}\rangle|\rho^{3,U}_{z_2,b}\rangle + \frac{1}{\sqrt{2}}\sum_{x_1,x_2=0}^{1}U(a)_{x_1x_2,z_1z_2}|\rho^{2,U}_{x_1,a}\rangle|\rho^{4,U}_{x_2,b}\rangle \tag{7.49}$$

for $z_1, z_2, a, b \in \{0, 1\}$. There are no N-particle frustration-free states on G_U for $N \geq 3$, i.e.,

$$\lambda^1_N(G_U) > 0 \quad \textit{for } N \geq 3.$$

We view the nodes labeled $\alpha, \beta, \gamma, \delta$ in Figure **??** as "input" nodes and those labeled $\epsilon, \zeta, \eta, \theta$ as "output nodes". Each of the states $|\rho^{i,U}_{x,y}\rangle$ is associated with one of the nodes, depending on the values of $i \in \{1, 2, 3, 4\}$ and $x \in \{0, 1\}$. For example, the states $|\rho^{1,U}_{0,0}\rangle$ and $|\rho^{1,U}_{0,1}\rangle$ are associated with input node α since they both have nonzero amplitude on vertices of the gate graph that are associated with α (and zero amplitude on vertices associated with other labeled nodes).

The two-particle state $\mathrm{Sym}(|T^{U}_{z_1,a,z_2,b}\rangle)$ is a superposition of a term

$$\mathrm{Sym}\left(\frac{1}{\sqrt{2}}|\rho^{1,U}_{z_1,a}\rangle|\rho^{3,U}_{z_2,b}\rangle\right)$$

with both particles located on vertices corresponding to input nodes and a term

$$\mathrm{Sym}\left(\frac{1}{\sqrt{2}}\sum_{x_1,x_2\in\{0,1\}} U(a)_{x_1x_2,z_1z_2}|\rho^{2,U}_{x_1,a}\rangle|\rho^{4,U}_{x_2,b}\rangle\right)$$

with both particles on vertices corresponding to output nodes. The two-qubit gate $U(a)$ is applied as the particles move from input nodes to output nodes.

7.2.2.2 Boundary gadget

The *boundary gadget* is shown in Figure **??**. This gate diagram is obtained from Figure **??** (with $\tilde{U} = \mathbb{I}$) by adding self-loops. The adjacency matrix is

$$A(G_{\mathrm{bnd}}) = A(G_{\mathrm{CNOT}_{12}}) + h_{\mathcal{S}}$$

where

$$h_{\mathcal{S}} = \sum_{z=0}^{1}(|1,z,1\rangle\langle 1,z,1|\otimes\mathbb{I}_j + |2,z,5\rangle\langle 2,z,5|\otimes\mathbb{I}_j + |3,z,1\rangle\langle 3,z,1|\otimes\mathbb{I}_j).$$

The single-particle ground states (with energy e_1) are superpositions of the states $|\rho^{i,U}_{z,a}\rangle$ from Lemma 17 that are in the nullspace of $h_{\mathcal{S}}$. Note that

$$\langle\rho^{j,U}_{x,b}|h_{\mathcal{S}}|\rho^{i,U}_{z,a}\rangle = \delta_{a,b}\delta_{x,z}\left(\delta_{i,1}\delta_{j,1} + \delta_{i,2}\delta_{j,2} + \delta_{i,3}\delta_{j,3}\right)\frac{1}{8}\cdot\frac{1}{8}$$

(one factor of $\frac{1}{8}$ comes from the normalization in equations (7.46)–(7.47) and the other factor comes from the normalization in equation (7.15)), so the only single-particle ground states are

$$|\rho^{\mathrm{bnd}}_{z,a}\rangle = |\rho^{4,U}_{z,a}\rangle$$

with $z,a\in\{0,1\}$. Thus there are no two- (or more) particle frustration-free states, because no superposition of the states (7.48) lies in the subspace

$$\mathrm{span}\{\mathrm{Sym}(|\rho^{4,U}_{z,a}\rangle|\rho^{4,U}_{x,b}\rangle)\colon z,a,x,b\in\{0,1\}\}$$

of states with single-particle reduced density matrices in the ground space of $A(G_{\mathrm{bnd}})$. We summarize these results as follows.

Lemma 18. *The smallest eigenvalue of $A(G_{bnd})$ is e_1, with corresponding eigenvectors*

$$|\rho^{bnd}_{z,a}\rangle = \frac{1}{\sqrt{8}}|\psi^{4}_{z,a}\rangle - \frac{1}{\sqrt{8}}|\psi^{8}_{z,a}\rangle - \sqrt{\frac{3}{8}}\sum_{x=0,1}|\chi^{x(z\oplus x)}_{4,a}\rangle. \tag{7.50}$$

There are no frustration-free states with two or more particles, i.e., $\lambda^1_N(G_{bnd}) > 0$ for $N\geq 2$.

7.2.3 Gate graph for a given circuit

For any n-qubit, M-gate verification circuit $\mathcal{C}_X$ of the form described above, we associate a gate graph G_X. The gate diagram for G_X is built using the gadgets described in Section **??**; specifically, we use M two-qubit gadgets and $2(n-1)$ boundary gadgets. Since each two-qubit gadget and each boundary gadget contains 32 diagram elements, the total number of diagram elements in G_X is $R = 32(M + 2n - 2)$.

We now present the construction of the gate diagram for G_X. We also describe some gate graphs obtained as intermediate steps that are used in our analysis in Section **??**. The reader may find this description easier to follow by looking ahead to Figure **??**, which illustrates this construction for a specific 3-qubit circuit.

1. **Draw a grid** with columns labeled $j = 0, 1, \ldots, M+1$ and rows labeled $i = 1, \ldots, n$ (this grid is only used to help describe the diagram).

2. **Place gadgets in the grid to mimic the quantum circuit.** For each $j = 1, \ldots, M$, place a gadget for the two-qubit gate U_j between rows 1 and $s(j)$ in the jth column. Place boundary gadgets in rows $i = 2, \ldots, n$ of column 0 and in the same rows of column $M+1$. Write G_1 for the gate graph associated with the resulting diagram.

3. **Connect the nodes within each row.** First add edges connecting the nodes in rows $i = 2, \ldots, n$; call the resulting gate graph G_2. Then add edges connecting the nodes in row 1; call the resulting gate graph G_3.

4. **Add self-loops to the boundary gadgets.** In this step we add self-loops to enforce initialization of ancillas (at the beginning) and the proper output of the circuit (at the end). For each row $k = n_{\text{in}}+1, \ldots, n$, add a self-loop to node δ (as shown in Figure **??**) of the corresponding boundary gadget in column $r = 0$, giving the gate diagram for G_4. Finally, add a self-loop to node α of the boundary gadget (as in Figure **??**) in row 2 and column $M+1$, giving the gate diagram for G_X.

Figure **??** illustrates the step-by-step construction of G_X using a simple 3-qubit circuit with four gates

$$\mathrm{CNOT}_{12}\,(\mathrm{CNOT}_{13} HT \otimes \mathbb{I})\,\mathrm{CNOT}_{21}\mathrm{CNOT}_{13}.$$

In this example, two of the qubits are input qubits (so $n_{\text{in}} = 2$), while the third qubit is an ancilla initialized to $|0\rangle$. Following the convention described in Section **??**, we take qubit 2 to be the output qubit. (In this example the circuit is not meant to compute anything interesting; its only purpose is to illustrate our method of constructing a gate graph).

We made some choices in designing this circuit-to-gate graph mapping that may seem arbitrary (e.g., we chose to place boundary gadgets in each row except the first). We have tried to achieve a balance between simplicity of description and ease of analysis, but we expect that other choices could be made to work.

7.2.3.1 Notation for G_X

We now introduce some notation that allows us to easily refer to a subset $\mathcal{L}$ of the diagram elements in the gate diagram for G_X.

Recall from Section **??** that each two-qubit gate gadget and each boundary gadget is composed of 32 diagram elements. This can be seen by looking at Figure **??** and noting (from Figure **??**) that each move-together gadget comprises 6 diagram elements.

For each of the two-qubit gate gadgets in the gate diagram for G_X, we focus our attention on the four diagram elements labeled 1–4 in Figure **??**. In total there are $4M$ such diagram elements in the gate diagram for G_X: in each column $j \in \{1, \ldots, M\}$ there are two in row 1 and two in row $s(j)$. When $U_j \in \{\mathrm{CNOT}_{1s(j)}, \mathrm{CNOT}_{1s(j)}\left(H \otimes \mathbb{I}\right), \mathrm{CNOT}_{1s(j)}\left(HT \otimes \mathbb{I}\right)\}$ the diagram elements labeled $1, 2$ are in row 1 and those labeled $3, 4$ are in row $s(j)$; when $U_j = \mathrm{CNOT}_{s(j)1}$ those labeled $1, 2$ are in row $s(j)$ and those labeled $3, 4$ are in row 1. We denote these diagram elements by triples (i, j, d). Here i and j indicate (respectively) the row and column of the grid in which the diagram element is found, and d indicates whether it is the leftmost ($d = 0$) or rightmost ($d = 1$) diagram element in this row and column. We define

$$\mathcal{L}_{\mathrm{gates}} = \{(i, j, d) : i \in \{1, s(j)\},\ j \in [M],\ d \in \{0, 1\}\} \tag{7.51}$$

to be the set of all such diagram elements.

For example, in Figure **??** the first gate is

$$U_1 = \mathrm{CNOT}_{13},$$

so the gadget from Figure **??** (with $\tilde{U} = 1$) appears between rows 1 and 3 in the first column. The diagram elements labeled $1, 2, 3, 4$ from Figure **??** are denoted by $(1, 1, 0), (1, 1, 1), (3, 1, 0), (3, 1, 1)$, respectively. The second gate in Figure **??** is $U_2 = \mathrm{CNOT}_{21}$, so the gadget from Figure **??** (with $\tilde{U} = 1$) appears between rows 2 and 1; in this case the diagram elements labeled $1, 2, 3, 4$ in Figure **??** are denoted by $(2, 2, 0), (2, 2, 1), (1, 2, 0), (1, 2, 1)$, respectively.

We also define notation for the boundary gadgets in G_X. For each boundary gadget. we focus on a single diagram element, labeled 4 in Figure **??**. For the left hand-side and right-hand side boundary gadgets, respectively, we denote these diagram elements as

$$\mathcal{L}_{\mathrm{in}} = \{(i, 0, 1)\colon i \in \{2, \ldots, n\}\} \tag{7.52}$$
$$\mathcal{L}_{\mathrm{out}} = \{(i, M+1, 0)\colon i \in \{2, \ldots, n\}\}\,. \tag{7.53}$$

Definition 8. Let $\mathcal{L}$ be the set of diagram elements

$$\mathcal{L} = \mathcal{L}_{\mathrm{in}} \cup \mathcal{L}_{\mathrm{gates}} \cup \mathcal{L}_{\mathrm{out}}$$

where $\mathcal{L}_{\mathrm{in}}$, $\mathcal{L}_{\mathrm{gates}}$, and $\mathcal{L}_{\mathrm{out}}$ are given by equations (7.52), (7.51), and (7.53), respectively.

Finally, it is convenient to define a function F that describes horizontal movement within the rows of the gate diagram for G_X. The function F takes as input a two-qubit gate $j \in [M]$, a qubit $i \in \{2, \ldots, n\}$, and a single bit and outputs a diagram element from the set $\mathcal{L}$. If the bit is 0 then F outputs the diagram element in row i that appears in a column $0 \leq k < j$ with k maximal (i.e., the closest diagram element in row i to the left of column j):

$$F(i, j, 0) = \begin{cases} (i, k, 1) & \text{where } 1 \leq k < j \text{ is the largest } k \text{ such that } s(k) = i\text{, if it exists} \\ (i, 0, 1) & \text{otherwise.} \end{cases} \tag{7.54}$$

On the other hand, if the bit is 1, then F outputs the diagram element in row i that appears in a column $j < k \leq M+1$ with k minimal (i.e., the closest diagram element in row i to the right of column j).

$$F(i,j,1) = \begin{cases} (i,k,0) & \text{where } j < k \leq M \text{ is the smallest } k \text{ such that } s(k) = j, \text{ if it exists} \\ (i, M+1, 0) & \text{otherwise.} \end{cases} \tag{7.55}$$

7.2.3.2 Occupancy constraints graph

In this Section we define an occupancy constraints graph $G_X oc$. Along with G_X and the number of particles n, this determines a subspace $\mathcal{I}(G_X, G_X oc, n) \subset \mathcal{Z}_n(G_X)$ through equation (**??**). We will see in Section **??** how low-energy states of the Bose-Hubbard model that live entirely within this subspace encode computations corresponding to the quantum circuit $\mathcal{C}_X$. This fact is used in the proof of Theorem **??**, which shows that the smallest eigenvalue $\lambda_n^1(G_X, G_X oc)$ of

$$H(G_X, G_X oc, n) = H(G_X, n)\big|_{\mathcal{I}(G_X, G_X oc, n)}$$

is related to the maximum acceptance probability of the circuit.

We encode quantum data in the locations of n particles in the graph G_X as follows. Each particle encodes one qubit and is located in one row of the graph G_X. Since all two-qubit gates in $\mathcal{C}_X$ involve the first qubit, the location of the particle in the first row determines how far along the computation has proceeded. We design the occupancy constraints graph to ensure that low-energy states of $H(G_X, G_X oc, n)$ have exactly one particle in each row (since there are n particles and n rows), and so that the particles in rows $2, \ldots, n$ are not too far behind or ahead of the particle in the first row. To avoid confusion, we emphasize that not *all* states in the subspace $\mathcal{I}(G_X, G_X oc, n)$ have the desired properties—for example, there are states in this subspace with more than one particle in a given row. We see in the next Section that states with low energy for $H(G_X, n)$ that also satisfy the occupancy constraints (i.e., low-energy states of $H(G_X, G_X oc, n)$) have the desired properties.

We now define $G_X oc$, which is a simple graph with a vertex for each diagram element in G_X. Each edge in $G_X oc$ places a constraint on the locations of particles in G_X. The graph $G_X oc$ only has edges between diagram elements in the set $\mathcal{L}$ from Definition 8; we define the edge set $E(G_X oc)$ by specifying pairs of diagram elements $L_1, L_2 \in \mathcal{L}$. We also indicate (in bold) the reason for choosing the constraints, which will become clearer in Section **??**.

1. **No two particles in the same row.** For each $i \in [n]$ we add constraints between diagram elements $(i,j,c) \in \mathcal{L}$ and $(i,k,d) \in \mathcal{L}$ in row i but in different columns, i.e.,

$$\{(i,j,c), (i,k,d)\} \in E(G_X oc) \text{ whenever } j \neq k. \tag{7.56}$$

2. **Synchronization with the particle in the first row.** For each $j \in [M]$ we add constraints between row 1 and row $s(j)$:

$$\{(1,j,c), (s(j),k,d)\} \in E(G_X oc) \text{ whenever } k \neq j \text{ and } (s(j),k,d) \neq F(s(j),j,c).$$

For each $j \in [M]$ we also add constraints between row 1 and rows $i \in [n] \setminus \{1, s(j)\}$:

$$\{(1,j,c), (i,k,d)\} \in E(G_X oc) \text{ whenever } (i,k,d) \notin \{F(i,j,0), F(i,j,1)\}.$$

7.3 Proof of QMA-hardness for MPQW ground energy

Theorem **??** bounds the smallest eigenvalue $\lambda_n^1(G_X, G_X oc)$ of $H(G_X, G_X oc, n)$. To prove the Theorem, we investigate a sequence of Hamiltonians starting with $H(G_1, n)$ and $H(G_1, G_X oc, n)$ and then work our way up to the Hamiltonian $H(G_X, G_X oc, n)$ by adding positive semidefinite terms.

For each Hamiltonian we consider, we solve for the nullspace and the smallest nonzero eigenvalue. To go from one Hamiltonian to the next, we use the following "Nullspace Projection Lemma," which was used (implicitly) in reference [**?**]. The Lemma bounds the smallest nonzero eigenvalue $\gamma(H_A + H_B)$ of a sum of positive semidefinite Hamiltonians H_A and H_B using knowledge of the smallest nonzero eigenvalue $\gamma(H_A)$ of H_A and the smallest nonzero eigenvalue $\gamma(H_B|_S)$ of the restriction of H_B to the nullspace S of H_A.

We prove the Lemma in Section **??**. When we apply this Lemma, we are usually interested in an asymptotic limit where $c, d \ll \|H_B\|$ and the right-hand side of (**??**) is $\Omega(\frac{cd}{\|H_B\|})$.

Our proof strategy, using repeated applications of the Nullspace Projection Lemma, is analogous to that of reference [**?**], where the so-called Projection Lemma was used similarly. Our technique has the advantage of not requiring the terms we add to our Hamiltonian to have "unphysical" problem-size dependent coefficients (it also has this advantage over the method of perturbative gadgets [**?**, **?**]). This allows us to prove results about the "physically realistic" Bose-Hubbard Hamiltonian. A similar technique based on Kitaev's Geometric Lemma was used recently in reference [**?**] (however, that method is slightly more computation intensive, requiring a lower bound on $\gamma(H_B)$ as well as bounds on $\gamma(H_A)$ and $\gamma(H_B|_S)$).

7.3.1 Single-particle ground-states

We begin by discussing the graphs

$$G_1, G_2, G_3, G_4, G_X$$

(as defined in Section **??**; see Figure **??**) in more detail and deriving some properties of their adjacency matrices.

The graph G_1 has a component for each of the two-qubit gates $j \in [M]$, for each of the boundary gadgets $i = 2, \ldots, n$ in column 0, and for each of the boundary gadgets $i = 2, \ldots, n$ in column $M + 1$. In other words

$$G_1 = \underbrace{\left(\bigcup_{i=2}^{n} G_{\mathrm{bnd}}\right)}_{\text{left boundary}} \cup \underbrace{\left(\bigcup_{j=1}^{M} G_{U_j}\right)}_{\text{two-qubit gates}} \cup \underbrace{\left(\bigcup_{i=2}^{n} G_{\mathrm{bnd}}\right)}_{\text{right boundary}}. \tag{7.57}$$

We use our knowledge of the adjacency matrices of the components G_{bnd} and G_{U_j} to understand the ground space of $A(G_1)$. Recall (from Section **??**) that the smallest eigenvalue of $A(G_{U_j})$ is

$$e_1 = -1 - 3\sqrt{2}$$

(with degeneracy 16) which is also the smallest eigenvalue of $A(G_{\mathrm{bnd}})$ (with degeneracy 4). For each diagram element $L \in \mathcal{L}$ and pair of bits $z, a \in \{0, 1\}$ there is an eigenstate $|\rho_{z,a}^L\rangle$ of

$A(G_1)$ with this minimal eigenvalue e_1. In total we get sixteen eigenstates

$$|\rho_{z,a}^{(1,j,0)}\rangle, |\rho_{z,a}^{(1,j,1)}\rangle, |\rho_{z,a}^{(s(j),j,0)}\rangle, |\rho_{z,a}^{(s(j),j,1)}\rangle, \quad z, a \in \{0, 1\}$$

for each two-qubit gate $j \in [M]$, four eigenstates

$$|\rho_{z,a}^{(i,0,1)}\rangle, \quad z, a \in \{0, 1\}$$

for each boundary gadget $i \in \{2, \ldots, n\}$ in column 0, and four eigenstates

$$|\rho_{z,a}^{(i,M+1,0)}\rangle, \quad z, a \in \{0, 1\}$$

for each boundary gadget $i \in \{2, \ldots, n\}$ in column $M + 1$. The set

$$\left\{|\rho_{z,a}^{L}\rangle \colon z, a \in \{0, 1\},\ L \in \mathcal{L}\right\}$$

is an orthonormal basis for the ground space of $A(G_1)$.

We write the adjacency matrices of G_2, G_3, G_4, and G_X as

$$A(G_2) = A(G_1) + h_1 \qquad A(G_4) = A(G_3) + \sum_{i=n_{\text{in}}+1}^{n} h_{\text{in},i}$$
$$A(G_3) = A(G_2) + h_2 \qquad A(G_X) = A(G_4) + h_{\text{out}}.$$

From step 3 of the construction of the gate diagram in Section **??**, we see that h_1 and h_2 are both sums of terms of the form

$$(|q, z, t\rangle + |q', z, t'\rangle)\,(\langle q, z, t| + \langle q', z, t'|) \otimes \mathbb{I}_j,$$

where h_1 contains a term for each edge in rows $2, \ldots, n$ and h_2 contains a term for each of the $2(M-1)$ edges in the first row. The operators

$$h_{\text{in},i} = |(i,0,1),1,7\rangle\langle(i,0,1),1,7| \otimes \mathbb{I} \quad h_{\text{out}} = |(2,M+1,0),0,5\rangle\langle(2,M+1,0),0,5| \otimes \mathbb{I} \tag{7.58}$$

correspond to the self-loops added in the gate diagram in step 4 of Section **??**.

We prove that G_1, G_2, G_3, G_4, and G_X are e_1-gate graphs.

Lemma 19. *The smallest eigenvalues of G_1, G_2, G_3, G_4 and G_X are*

$$\mu(G_1) = \mu(G_2) = \mu(G_3) = \mu(G_4) = \mu(G_X) = e_1.$$

Proof. We showed in the above discussion that $\mu(G_1) = e_1$. The adjacency matrices of G_2, G_3, G_4, and G_X are obtained from that of G_1 by adding positive semidefinite terms (h_1, h_2, $h_{\text{in},i}$, and h_{out} are all positive semidefinite). It therefore suffices to exhibit an eigenstate $|\varrho\rangle$ of $A(G_1)$ with

$$h_1|\varrho\rangle = h_2|\varrho\rangle = h_{\text{in},i}|\varrho\rangle = h_{\text{out}}|\varrho\rangle = 0$$

(for each $i \in \{n_{\text{in}} + 1, \ldots, n\}$). There are many states $|\varrho\rangle$ satisfying these conditions; one example is

$$|\varrho\rangle = |\rho_{0,0}^{(1,1,0)}\rangle$$

which is supported on vertices where h_1, h_2, $h_{\text{in},i}$, and h_{out} have no support. □

7.3.1.1 Multi-particle Hamiltonian

We now outline the sequence of Hamiltonians considered in the following Sections and describe the relationships between them. As a first step, in Section **??** we exhibit a basis $\mathcal{B}_n$ for the nullspace of $H(G_1, n)$ and we prove that its smallest nonzero eigenvalue is lower bounded by a positive constant. We then discuss the restriction

$$H(G_1, G_X oc, n) = H(G_1, n)\big|_{\mathcal{I}(G_1, G_X oc, n)} \tag{7.59}$$

in Section **??**, where we prove that a subset $\mathcal{B}_{\text{legal}} \subset \mathcal{B}_n$ is a basis for the nullspace of (7.59), and that its smallest nonzero eigenvalue is also lower bounded by a positive constant.

For the remainder of the proof we use the Nullspace Projection Lemma (Lemma **??**) four times, using the decompositions

$$H(G_2, G_X oc, n) = H(G_1, G_X oc, n) + H_1\big|_{\mathcal{I}(G_2, G_X oc, n)} \tag{7.60}$$

$$H(G_3, G_X oc, n) = H(G_2, G_X oc, n) + H_2\big|_{\mathcal{I}(G_3, G_X oc, n)} \tag{7.61}$$

$$H(G_4, G_X oc, n) = H(G_3, G_X oc, n) + \sum_{i=n_{\text{in}}+1}^{n} H_{\text{in},i}\big|_{\mathcal{I}(G_4, G_X oc, n)} \tag{7.62}$$

$$H(G_X, G_X oc, n) = H(G_4, G_X oc, n) + H_{\text{out}}\big|_{\mathcal{I}(G_X, G_X oc, n)} \tag{7.63}$$

where

$$H_1 = \sum_{w=1}^{n} h_1^{(w)} \qquad H_{\text{in},i} = \sum_{w=1}^{n} h_{\text{in},i}^{(w)} \qquad H_2 = \sum_{w=1}^{n} h_2^{(w)} \qquad H_{\text{out}} = \sum_{w=1}^{n} h_{\text{out}}^{(w)}$$

are all positive semidefinite, with $h_1, h_2, h_{\text{in},i}, h_{\text{out}}$ as defined in Section **??**. Note that in writing equations (7.60), (7.61), (7.62), and (7.63), we have used the fact (from Lemma 19) that the adjacency matrices of the graphs we consider all have the same smallest eigenvalue e_1. Also note that

$$\mathcal{I}\left(G_i, G_X oc, n\right) = \mathcal{I}\left(G_X, G_X oc, n\right)$$

for $i \in [4]$ since the gate diagrams for each of the graphs G_1, G_2, G_3, G_4 and G_X have the same set of diagram elements.

Let S_k be the nullspace of $H(G_k, G_X oc, n)$ for $k = 1, 2, 3, 4$. Since these positive semidefinite Hamiltonians are related by adding positive semidefinite terms, their nullspaces satisfy

$$S_4 \subseteq S_3 \subseteq S_2 \subseteq S_1 \subseteq \mathcal{I}\left(G_X, G_X oc, n\right).$$

We solve for $S_1 = \text{span}(\mathcal{B}_{\text{legal}})$ in Section **??** and we characterize the spaces S_2, S_3, and S_4 in Section **??** in the course of applying our strategy.

For example, to use the Nullspace Projection Lemma to lower bound the smallest nonzero eigenvalue of $H(G_2, G_X oc, n)$, we consider the restriction

$$\left(H_1\big|_{\mathcal{I}(G_2, G_X oc, n)}\right)\Big|_{S_1} = H_1\big|_{S_1}. \tag{7.64}$$

We also solve for S_2, which is equal to the nullspace of (7.64). To obtain the corresponding lower bounds on the smallest nonzero eigenvalues of $H(G_k, G_X oc, n)$ for $k = 2, 3, 4$ and $H(G_X, G_X oc, n)$, we consider restrictions

$$H_2\big|_{S_2}, \sum_{i=n_{\text{in}}+1}^{n} H_{\text{in},i}\big|_{S_3}, \quad \text{and} \quad H_{\text{out}}\big|_{S_4}.$$

Analyzing these restrictions involves extensive computation of matrix elements. To simplify and organize these computations, we first compute the restrictions of each of these operators to the space S_1. We present the results of this computation in Section **??**; details of the calculation can be found in Section **??**. In Section **??** we proceed with the remaining computations and apply the Nullspace Projection Lemma three times using equations (7.60), (7.61), and (7.62). Finally, in Section **??** we apply the Lemma again using equation (7.63) and we prove Theorem **??**.

7.3.2 Configurations

In this Section we use Lemma 12 to solve for the nullspace of $H(G_1, n)$, i.e., the n-particle frustration-free states on G_1. Lemma 12 describes how frustration-free states for G_1 are built out of frustration-free states for its components.

To see how this works, consider the example from Figure **??**. In this example, with $n = 3$, we construct a basis for the nullspace of $H(G_1, 3)$ by considering two types of eigenstates. First, there are frustration-free states

$$\text{Sym}(|\rho^{L_1}_{z_1,a_1}\rangle|\rho^{L_2}_{z_2,a_2}\rangle|\rho^{L_3}_{z_3,a_3}\rangle) \tag{7.65}$$

where $L_k = (i_k, j_k, d_k) \in \mathcal{L}$ belong to different components of G_1. That is to say, $j_w \neq j_t$ unless $j_w = j_t \in \{0, 5\}$, in which case $i_w \neq i_t$ (in this case the particles are located either at the left or right boundary, in different rows of G_1). There are also frustration-free states where two of the three particles are located in the same two-qubit gadget $J \in [M]$ and one of the particles is located in a diagram element L_1 from a different component of the graph. These states have the form

$$\text{Sym}(|T^J_{z_1,a_1,z_2,a_2}\rangle|\rho^{L_1}_{z_3,a_3}\rangle) \tag{7.66}$$

where

$$|T^J_{z_1,a_1,z_2,a_2}\rangle = \frac{1}{\sqrt{2}}|\rho^{(1,J,0)}_{z_1,a_1}\rangle|\rho^{(s(J),J,0)}_{z_2,a_2}\rangle + \frac{1}{\sqrt{2}}\sum_{x_1,x_2\in\{0,1\}} U_J(a_1)_{x_1x_2,z_1z_2}|\rho^{(1,J,1)}_{x_1,a_1}\rangle|\rho^{(s(J),J,1)}_{x_2,a_2}\rangle \tag{7.67}$$

and $L_1 = (i, j, k) \in \mathcal{L}$ satisfies $j \neq J$. Each of the states (7.65) and (7.66) is specified by 6 "data" bits $z_1, z_2, z_3, a_1, a_2, a_3 \in \{0, 1\}$ and a "configuration" indicating where the particles are located in the graph. The configuration is specified either by three diagram elements $L_1, L_2, L_3 \in \mathcal{L}$ from different components of G_1 or by a two-qubit gate $J \in [M]$ along with a diagram element $L_1 \in \mathcal{L}$ from a different component of the graph.

We now define the notion of a configuration for general n. Informally, we can think of an n-particle configuration as a way of placing n particles in the graph G_1 subject to the following restrictions. We first place each of the n particles in a component of the graph, with the restriction that no boundary gadget may contain more than one particle and no two-qubit gadget may contain more than two particles. For each particle on its own in a component (i.e., in a component with no other particles), we assign one of the diagram elements $L \in \mathcal{L}$ associated to that component. We therefore specify a configuration by a set of two-qubit gadgets $J_1, \ldots, J_Y$ that contain two particles, along with a set of diagram elements $L_k \in \mathcal{L}$ that give the locations of the remaining $n - 2Y$ particles. We choose to order the Js and the Ls so that each configuration is specified by a unique tuple $(J_1, \ldots, J_Y, L_1, \ldots, L_{n-2Y})$. For concreteness, we use the lexicographic order on diagram elements in the set $\mathcal{L}$: $L_A = (i_A, j_A, d_A)$ and $L_B = (i_B, j_B, d_B)$ satisfy $L_A < L_B$ iff either $i_A < i_B$, or $i_A = i_B$ and $j_A < j_B$, or $(i_A, j_A) = (i_B, j_B)$ and $d_A < d_B$.

Definition 9 (**Configuration**)**.** An n-particle configuration on the gate graph G_1 is a tuple

$$(J_1, \ldots, J_Y, L_1, \ldots, L_{n-2Y})$$

with $Y \in \{0, \ldots, \lfloor \frac{n}{2} \rfloor\}$, ordered integers

$$1 \leq J_1 < J_2 < \cdots < J_Y \leq M,$$

and lexicographically ordered diagram elements

$$L_1 < L_2 < \cdots < L_{n-2Y}, \qquad L_k = (i_k, j_k, d_k) \in \mathcal{L}.$$

We further require that each L_k is from a different component of G_1, i.e.,

$$j_w = j_t \quad \Longrightarrow \quad j_w \in \{0, M+1\} \text{ and } i_w \neq i_t,$$

and we require that $j_u \neq J_v$ for all $u \in [n - 2Y]$ and $v \in [Y]$.

In Figure **??** we give some examples of configurations (for the example from Figure **??** with $n = 3$) and we introduce a diagrammatic notation for them.

For any configuration and n-bit strings $\vec{z}$ and $\vec{a}$, there is a state in the nullspace of $H(G_1, n)$, given by

$$\mathrm{Sym}(|T^{J_1}_{z_1,a_1,z_2,a_2}\rangle \ldots |T^{J_Y}_{z_{2Y-1},a_{2Y-1},z_{2Y},a_{2Y}}\rangle |\rho^{L_1}_{z_{2Y+1},a_{2Y+1}}\rangle \ldots |\rho^{L_{n-2Y}}_{z_n,a_n}\rangle). \tag{7.68}$$

The ordering in the definition of a configuration ensures that each distinct choice of configuration and n-bit strings $\vec{z}, \vec{a}$ gives a different state.

Definition 10. Let $\mathcal{B}_n$ be the set of all states of the form (7.68), where $(J_1, \ldots, J_Y, L_1, \ldots, L_{n-2Y})$ is a configuration and $\vec{z}, \vec{a} \in \{0,1\}^n$.

Lemma 20. *The set $\mathcal{B}_n$ is an orthonormal basis for the nullspace of $H(G_1, n)$. Furthermore,*

$$\gamma(H(G_1, n)) \geq \mathcal{K}_0 \tag{7.69}$$

where $\mathcal{K}_0 \in (0, 1]$ is an absolute constant.

Proof. Each component of G_1 is either a two-qubit gadget or a boundary gadget (see equation (7.57)). The single-particle states of $A(G_1)$ with energy e_1 are the states $|\rho^L_{z,a}\rangle$ for $L \in \mathcal{L}$ and $z, a \in \{0, 1\}$, as discussed in Section **??**. Each of these states has support on only one component of G_1. In addition, G_1 has a two-particle frustration-free state for each two-qubit gadget $J \in [M]$ and bits z, a, x, b, namely $\mathrm{Sym}(|T^J_{z,a,x,b}\rangle)$. Furthermore, no component of G_1 has any three- (or more) particle frustration-free states. Using these facts and applying Lemma 12, we see that $\mathcal{B}_n$ spans the nullspace of $H(G_1, n)$.

Lemma 12 also expresses each eigenvalue of $H(G_1, n)$ as a sum of eigenvalues for its components. We use this fact to obtain the desired lower bound on the smallest nonzero eigenvalue. Our analysis proceeds on a case-by-case basis, depending on the occupation numbers for each component of G_1 (the values $N_1, \ldots, N_k$ in Lemma 12).

First consider any set of occupation numbers where some two-qubit gate gadget $J \in [M]$ contains 3 or more particles. By Lemma **??** and Lemma 12, any such eigenvalue is at least $\lambda^1_3(G_{U_J})$, which is a positive constant by Lemma 17. Next consider a case where some boundary gadget contains more than one particle. The corresponding eigenvalues are similarly lower bounded by $\lambda^1_2(G_{\mathrm{bnd}})$, which is also a positive constant by Lemma 18. Finally, consider a set of occupation numbers where each two-qubit gadget contains at most two particles and each boundary gadget contains at most one particle. The smallest eigenvalue with such a set of occupation numbers is zero. The smallest nonzero eigenvalue is either

$$\gamma(H(G_{U_J}, 1)),\ \gamma(H(G_{U_J}, 2)) \text{ for some } J \in [M], \text{ or } \gamma(H(G_{\mathrm{bnd}}, 1)).$$

However, these quantities are at least some positive constant since $H(G_{U_J}, 1)$, $H(G_{U_J}, 2)$, and $H(G_{\mathrm{bnd}}, 1)$ are nonzero constant-sized positive semidefinite matrices.

Now combining the lower bounds discussed above and using the fact that, for each $J \in [M]$, the two-qubit gate U_J is chosen from a fixed finite gate set (given in (**??**)), we see that $\gamma(H(G_1, n))$ is lower bounded by the positive constant

$$\min\{\lambda^1_3(G_U), \lambda^1_2(G_{\mathrm{bnd}}), \gamma(H(G_U, 1)), \gamma(H(G_U, 2)), \gamma(H(G_{\mathrm{bnd}}, 1)) \colon U \text{ is from the gate set } (\textbf{??})\}. \tag{7.70}$$

The condition $\mathcal{K}_0 \leq 1$ can be ensured by setting $\mathcal{K}_0$ to be the minimum of 1 and (7.70). □

Note that the constant $\mathcal{K}_0$ can in principle be computed using (7.70): each quantity on the right-hand side can be evaluated by diagonalizing a specific finite-dimensional matrix.

7.3.2.1 Legal configurations

In this section we define a subset of the n-particle configurations that we call legal configurations, and we prove that the subset of the basis vectors in $\mathcal{B}_n$ that have legal configurations spans the nullspace of $H(G_1, G_X oc, n)$.

We begin by specifying the set of legal configurations. Every legal configuration

$$(J_1, \ldots, J_Y, L_1, \ldots, L_{n-2Y})$$

has $Y \in \{0, 1\}$. The legal configurations with $Y = 0$ are

$$((1, j, d_1), F(2, j, d_2), F(3, j, d_3), \ldots, F(n, j, d_n)) \tag{7.71}$$

where $j \in [M]$ and where $\vec{d} = (d_1, \ldots, d_n)$ satisfies $d_i \in \{0,1\}$ and $d_1 = d_{s(j)}$. (Recall that the function F, defined in equations (7.54) and (7.55), describes horizontal movement of particles.) The legal configurations with $Y = 1$ are

$$(j, F(2,j,d_2), \ldots, F(s(j)-1, j, d_{s(j)-1}), F(s(j)+1, j, d_{s(j)+1}), \ldots, F(n,j,d_n)) \tag{7.72}$$

where $j \in \{1, \ldots, M\}$ and $d_i \in \{0,1\}$ for $i \in [n] \setminus \{1, s(j)\}$. Although the values d_1 and $d_{s(j)}$ are not used in equation (7.72), we choose to set them to

$$d_1 = d_{s(j)} = 2$$

for any legal configuration with $Y = 1$. In this way we identify the set of legal configurations with the set of pairs $j, \vec{d}$ with $j \in [M]$ and

$$\vec{d} = (d_1, d_2, d_3, \ldots, d_n)$$

satisfying

$$d_1 = d_{s(j)} \in \{0,1,2\} \quad \text{and} \quad d_i \in \{0,1\} \text{ for } i \notin \{1, s(j)\}.$$

The legal configuration is given by equation (7.71) if $d_1 = d_{s(j)} \in \{0,1\}$ and equation (7.72) if $d_1 = d_{s(j)} = 2$.

The examples in Figures **??**, **??**, and **??** show legal configurations whereas the examples in Figures **??**, **??**, and **??** are illegal. The legal examples correspond to $j = 1$, $\vec{d} = (1,1,1)$; $j = 2$, $\vec{d} = (2,2,0)$; and $j = 1$, $\vec{d} = (1,0,1)$, respectively. We now explain why the other examples are illegal. Looking at (7.72), we see that the configuration $(3,(2,0,1))$ depicted in Figure **??** is illegal since $F(2,3,0) = (2,2,1) \neq (2,0,1)$ and $F(2,3,1) = (2,4,0) \neq (2,0,1)$. The configuration in Figure **??** is illegal since there are two particles in the same row. Looking at equation (7.71), we see that the configuration $((1,1,1),(2,2,0),(3,5,0))$ in Figure **??** is illegal since $(3,5,0) \notin \{F(3,1,0), F(3,1,1)\} = \{(3,0,1),(3,3,0)\}$.

We now identify the subset of basis vectors $\mathcal{B}_{\text{legal}} \subset \mathcal{B}_n$ that have legal configurations. We write each such basis vector as

$$|j, \vec{d}, \vec{z}, \vec{a}\rangle = \begin{cases} \operatorname{Sym}\left(|\rho_{z_1,a_1}^{(1,j,d_1)}\rangle \displaystyle\bigotimes_{i=2}^{n} |\rho_{z_i,a_i}^{F(i,j,d_i)}\rangle\right) & d_1 = d_{s(j)} \in \{0,1\} \\ \operatorname{Sym}\left(|T^j_{z_1,a_1,z_{s(j)},a_{s(j)}}\rangle \displaystyle\bigotimes_{\substack{i=2 \\ i \neq s(j)}}^{n} |\rho_{z_i,a_i}^{F(i,j,d_i)}\rangle\right) & d_1 = d_{s(j)} = 2 \end{cases} \tag{7.73}$$

where $j, \vec{d}$ specifies the legal configuration and $\vec{z}, \vec{a} \in \{0,1\}^n$. (Note that the bits in $\vec{z}$ and $\vec{a}$ are ordered slightly differently than in equation (7.68); here the labeling reflects the indices of the encoded qubits).

Definition 11. Let

$$\mathcal{B}_{\text{legal}} = \left\{|j, \vec{d}, \vec{z}, \vec{a}\rangle : j \in [M],\ d_1 = d_{s(j)} \in \{0,1,2\} \text{ and } d_i \in \{0,1\} \text{ for } i \notin \{1, s(j)\},\ \vec{z}, \vec{a} \in \{0,1\}^n\right\}$$

and $\mathcal{B}_{\text{illegal}} = \mathcal{B}_n \setminus \mathcal{B}_{\text{illegal}}$.

The basis $\mathcal{B}_n = \mathcal{B}_{\text{legal}} \cup \mathcal{B}_{\text{illegal}}$ is convenient when considering the restriction to the subspace $\mathcal{I}(G_1, G_X oc, n)$. Letting Π_0 be the projector onto $\mathcal{I}(G_1, G_X oc, n)$, the following Lemma (proven in Section **??**) shows that the restriction

$$\Pi_0\big|_{\text{span}(\mathcal{B}_n)} \tag{7.74}$$

is diagonal in the basis $\mathcal{B}_n$. The Lemma also bounds the diagonal entries.

Lemma 21. *Let Π_0 be the projector onto $\mathcal{I}(G_1, G_X oc, n)$. For any $|j, \vec{d}, \vec{z}, \vec{a}\rangle \in \mathcal{B}_{legal}$, we have*

$$\Pi_0 |j, \vec{d}, \vec{z}, \vec{a}\rangle = |j, \vec{d}, \vec{z}, \vec{a}\rangle. \tag{7.75}$$

Furthermore, for any two distinct basis vectors $|\phi\rangle, |\psi\rangle \in \mathcal{B}_{illegal}$, we have

$$\langle\phi|\Pi_0|\phi\rangle \leq \frac{255}{256} \tag{7.76}$$

$$\langle\phi|\Pi_0|\psi\rangle = 0. \tag{7.77}$$

We use this Lemma to characterize the nullspace of $H(G_1, G_X oc, n)$ and bound its smallest nonzero eigenvalue.

Lemma 22. *The nullspace S_1 of $H(G_1, G_X oc, n)$ is spanned by the orthonormal basis $\mathcal{B}_{legal}$. Its smallest nonzero eigenvalue is*

$$\gamma(H(G_1, G_X oc, n)) \geq \frac{\mathcal{K}_0}{256} \tag{7.78}$$

where $\mathcal{K}_0 \in (0, 1]$ is the absolute constant from Lemma 20.

Proof. Recall from Section **??** that

$$H(G_1, G_X oc, n) = H(G_1, n)|_{\mathcal{I}(G_1, G_X oc, n)}.$$

Its nullspace is the space of states $|\kappa\rangle$ satisfying

$$\Pi_0|\kappa\rangle = |\kappa\rangle \quad \text{and} \quad H(G_1, n)|\kappa\rangle = 0$$

(recall that Π_0 is the projector onto $\mathcal{I}(G_1, G_X oc, n)$, the states satisfying the occupancy constraints). Since $\mathcal{B}_n$ is a basis for the nullspace of $H(G_1, n)$, to solve for the nullspace of $H(G_1, G_X oc, n)$ we consider the restriction (7.74) and solve for the eigenspace with eigenvalue 1. This calculation is simple because (7.74) is diagonal in the basis $\mathcal{B}_n$, according to Lemma 21. We see immediately from the Lemma that $\mathcal{B}_{\text{legal}}$ spans the nullspace of $H(G_1, G_X oc, n)$; we now show that Lemma 21 also implies the lower bound (7.78). Note that

$$\gamma(H(G_1, G_X oc, n)) = \gamma(\Pi_0 H(G_1, n) \Pi_0).$$

Let Π_{legal} and Π_{illegal} project onto the spaces spanned by $\mathcal{B}_{\text{legal}}$ and $\mathcal{B}_{\text{illegal}}$ respectively, so $\Pi_{\text{legal}} + \Pi_{\text{illegal}}$ projects onto the nullspace of $H(G_1, n)$. The operator inequality

$$H(G_1, n) \geq \gamma(H(G_1, n)) \cdot (1 - \Pi_{\text{legal}} - \Pi_{\text{illegal}})$$

implies

$$\Pi_0 H(G_1,n)\Pi_0 \geq \gamma(H(G_1,n)) \cdot \Pi_0(1-\Pi_{\text{legal}}-\Pi_{\text{illegal}})\Pi_0.$$

Since the operators on both sides of this inequality are positive semidefinite and have the same nullspace, their smallest nonzero eigenvalues are bounded as

$$\gamma(\Pi_0 H(G_1,n)\Pi_0) \geq \gamma(H(G_1,n)) \cdot \gamma(\Pi_0(1-\Pi_{\text{legal}}-\Pi_{\text{illegal}})\Pi_0).$$

Hence

$$\gamma(H(G_1,G_X oc,n)) = \gamma(\Pi_0 H(G_1,n)\Pi_0) \geq \mathcal{K}_0 \cdot \gamma(\Pi_0(1-\Pi_{\text{legal}}-\Pi_{\text{illegal}})\Pi_0) \tag{7.79}$$

where we used Lemma 20. From equations (7.76) and (7.77) we see that

$$\Pi_0|g\rangle = |g\rangle \quad \text{and} \quad \Pi_{\text{illegal}}|f\rangle = |f\rangle \qquad \Longrightarrow \qquad \langle f|g\rangle\langle g|f\rangle \leq \frac{255}{256}. \tag{7.80}$$

The nullspace of

$$\Pi_0\left(1-\Pi_{\text{legal}}-\Pi_{\text{illegal}}\right)\Pi_0 \tag{7.81}$$

is spanned by

$$\mathcal{B}_{\text{legal}} \cup \left\{|\tau\rangle \colon \Pi_0|\tau\rangle = 0\right\}.$$

To see this, note that (7.81) commutes with Π_0, and the space of $+1$ eigenvectors of Π_0 that are annihilated by (7.81) is spanned by $\mathcal{B}_{\text{legal}}$ (by Lemma 21). Any eigenvector $|g_1\rangle$ corresponding to the smallest nonzero eigenvalue of this operator therefore satisfies $\Pi_0|g_1\rangle = |g_1\rangle$ and $\Pi_{\text{legal}}|g_1\rangle = 0$, so

$$\gamma(\Pi_0(1-\Pi_{\text{legal}}-\Pi_{\text{illegal}})\Pi_0) = 1 - \langle g_1|\Pi_{\text{illegal}}|g_1\rangle \geq \frac{1}{256}$$

using equation (7.80). Plugging this into equation (7.79) gives the lower bound (7.78). □

We now consider

$$H_1|_{S_1}, H_2|_{S_1}, H_{\text{in},i}|_{S_1}, H_{\text{out}}|_{S_1} \tag{7.82}$$

where these operators are defined in Section 7.3.1.1 and

$$S_1 = \text{span}(\mathcal{B}_{\text{legal}})$$

is the nullspace of $H(G_1,G_X oc,n)$.

We specify the operators (7.82) by their matrix elements in an orthonormal basis for S_1. Although the basis $\mathcal{B}_{\text{legal}}$ was convenient in Section **??**, here we use a different basis in which the matrix elements of H_1 and H_2 are simpler. We define

$$|j,\vec{d},\text{In}(\vec{z}),\vec{a}\rangle = \sum_{\vec{x}\in\{0,1\}^n} \left(\langle\vec{x}|\bar{U}_{j,d_1}(a_1)|\vec{z}\rangle\right)|j,\vec{d},\vec{x},\vec{a}\rangle \tag{7.83}$$

where

$$\bar{U}_{j,d_1}(a_1) = \begin{cases} U_{j-1}(a_1)U_{j-2}(a_1)\ldots U_1(a_1) & \text{if } d_1 \in \{0,2\} \\ U_j(a_1)U_{j-1}(a_1)\ldots U_1(a_1) & \text{if } d_1 = 1. \end{cases} \tag{7.84}$$

In each of these states the quantum data (represented by the $\vec{x}$ register on the right-hand side) encodes the computation in which the unitary $\bar{U}_{j,d_1}(a_1)$ is applied to the initial n-qubit state $|\vec{z}\rangle$ (the notation $\mathrm{In}(\vec{z})$ indicates that $\vec{z}$ is the input). The vector $\vec{a}$ is only relevant insofar as its first bit a_1 determines whether or not each two-qubit unitary is complex conjugated; the other bits of $\vec{a}$ go along for the ride. Letting $\vec{z}, \vec{a} \in \{0,1\}^n$, $j \in [M]$, and

$$\vec{d} = (d_1, \ldots, d_n) \quad \text{with} \quad d_1 = d_{s(j)} \in \{0,1,2\} \quad \text{and} \quad d_i \in \{0,1\},\ i \notin \{1, s(j)\},$$

we see that the states (7.83) form an orthonormal basis for S_1. In Section **??** we compute the matrix elements of the operators (7.82) in this basis, which are reproduced below.

Roughly speaking, the nonzero off-diagonal matrix elements of the operator H_1 in the basis (7.83) occur between states $|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle$ and $|j, \vec{c}, \mathrm{In}(\vec{z}), \vec{a}\rangle$ where the legal configurations $j, \vec{d}$ and $j, \vec{c}$ are related by horizontal motion of a particle in one of the rows $i \in \{2, \ldots, n\}$.

Matrix elements of H_1

$$\langle k, \vec{c}, \mathrm{In}(\vec{x}), \vec{b}|H_1|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle = \delta_{k,j}\delta_{\vec{a},\vec{b}}\delta_{\vec{z},\vec{x}} \cdot \begin{cases} \frac{n-1}{64} & \vec{c} = \vec{d} \\ \frac{1}{64}\prod_{\substack{r=1 \\ r\neq i}}^{n} \delta_{d_r,c_r} & d_i \neq c_i \text{ for some } i \in [n] \setminus \{1, s(j)\} \\ \frac{1}{64\sqrt{2}} \prod_{\substack{r=2 \\ r\neq s(j)}}^{n} \delta_{d_r,c_r} & (c_1, d_1) \in \{(2,0),(0,2),(1,2),(2,1)\} \\ 0 & \text{otherwise.} \end{cases} \tag{7.85}$$

From this expression we see that $H_1|_{S_1}$ is block diagonal in the basis (7.83), with a block for each $\vec{z}, \vec{a} \in \{0,1\}^n$ and $j \in [M]$. Moreover, the submatrix for each block is the same. In Figure **??** we illustrate some of the off-diagonal matrix elements of $H_1|_{S_1}$ for the example from Figure **??**.

Next, we present the matrix elements of H_2.

Matrix elements of H_2

$$\begin{aligned} \langle k, \vec{c}, \mathrm{In}(\vec{x}), \vec{b}|H_2|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle = {} & f_{\mathrm{diag}(\vec{d},j)\cdot\delta_{j,k}\delta_{\vec{a},\vec{b}}\delta_{\vec{z},\vec{x}}\delta_{\vec{c},\vec{d}}} \\ & + \left(f_{\text{off-diag}}(\vec{c}, \vec{d}, j)\cdot\delta_{k,j-1} + f_{\text{off-diag}}(\vec{d}, \vec{c}, k)\cdot\delta_{k-1,j}\right)\delta_{\vec{a},\vec{b}}\delta_{\vec{z},\vec{x}} \end{aligned} \tag{7.86}$$

where

$$f_{\mathrm{diag}}(\vec{d}, j) = \begin{cases} 0 & d_1 = 0 \text{ and } j = 1, \text{ or } d_1 = 1 \text{ and } j = M \\ \frac{1}{128} & d_1 = 2 \text{ and } j \in \{1, M\} \\ \frac{1}{64} & \text{otherwise} \end{cases} \tag{7.87}$$

and

$$f_{\text{off-diag}}(\vec{c},\vec{d},j) = \left(\prod_{\substack{r=2\\ r\notin\{s(j-1),s(j)\}}}^{n} \delta_{d_r,c_r}\right) \cdot \begin{cases} \frac{1}{64\sqrt{2}} & (c_1, c_{s(j)}, d_1, d_{s(j-1)}) \in \{(2,0,0,0),(1,1,2,1)\} \\ \frac{1}{64} & (c_1, c_{s(j)}, d_1, d_{s(j-1)}) = (1,0,0,1) \\ \frac{1}{128} & (c_1, c_{s(j)}, d_1, d_{s(j-1)}) = (2,1,2,0) \\ 0 & \text{otherwise.} \end{cases} \tag{7.88}$$

This shows that $H_2|_{S_1}$ is block diagonal in the basis (7.83), with a block for each $\vec{z},\vec{a} \in \{0,1\}^n$. Also note that (in contrast with H_1) H_2 connects states with different values of j. In Figure **??** we illustrate some of the off-diagonal matrix elements of $H_2|_{S_1}$, for the example from Figure **??**.

Finally, we present the matrix elements of $H_{\text{in},i}$ (for $i \in \{n_{\text{in}}+1,\ldots,n\}$) and H_{out}:

Matrix elements of $H_{\text{in},i}$

For each ancilla qubit $i \in \{n_{\text{in}}+1,\ldots,n\}$, define $j_{\min,i} = \min\{j \in [M]\colon s(j)=i\}$ to be the index of the first gate in the circuit that involves this qubit (recall from Section **??** that we consider circuits where each ancilla qubit is involved in at least one gate). The operator $H_{\text{in},i}$ is diagonal in the basis (7.83), with entries

$$\langle j,\vec{d},\mathrm{In}(\vec{z}),\vec{a}|H_{\text{in},i}|j,\vec{d},\mathrm{In}(\vec{z}),\vec{a}\rangle = \begin{cases} \frac{1}{64} & j \le j_{\min,i},\ z_i = 1,\ \text{and } d_i = 0 \\ 0 & \text{otherwise.} \end{cases} \tag{7.89}$$

Matrix elements of H_{out}

Let $j_{\max} = \max\{j \in [M]\colon s(j) = 2\}$ be the index of the last gate $U_{j_{\max}}$ in the circuit that acts between qubits 1 and 2 (the output qubit). Then

$$\langle k,\vec{c},\mathrm{In}(\vec{x}),\vec{b}|H_{\text{out}}|j,\vec{d},\mathrm{In}(\vec{z}),\vec{a}\rangle = \delta_{j,k}\delta_{\vec{c},\vec{d}}\delta_{\vec{a},\vec{b}} \begin{cases} \langle\vec{x}|U_{\mathcal{C}_X}^\dagger(a_1)|0\rangle\langle 0|_2 U_{\mathcal{C}_X}(a_1)|\vec{z}\rangle\frac{1}{64} & j \ge j_{\max} \text{ and } d_2 = 1 \\ 0 & \text{otherwise.} \end{cases} \tag{7.90}$$

7.3.3 Frustration-Free states

Define the $(n-2)$-dimensional hypercubes

$$\mathcal{D}_k^j = \left\{(d_1,\ldots,d_n)\colon d_1 = d_{s(j)} = k,\, d_i \in \{0,1\} \text{ for } i \in [n]\setminus\{1,s(j)\}\right\}$$

for $j \in \{1,\ldots,M\}$ and $k \in \{0,1,2\}$, and the superpositions

$$|\mathrm{Cube}_k(j,\vec{z},\vec{a})\rangle = \frac{1}{\sqrt{2^{n-2}}}\sum_{\vec{d}\in\mathcal{D}_k^j}(-1)^{\sum_{i=1}^n d_i}\,|j,\vec{d},\mathrm{In}(\vec{z}),\vec{a}\rangle$$

for $k \in \{0,1,2\}$, $j \in [M]$, and $\vec{z}, \vec{a} \in \{0,1\}^n$. For each $j \in [M]$ and $\vec{z}, \vec{a} \in \{0,1\}^n$, let

$$|C(j,\vec{z},\vec{a})\rangle = \frac{1}{2}|\text{Cube}_0(j,\vec{z},\vec{a})\rangle + \frac{1}{2}|\text{Cube}_1(j,\vec{z},\vec{a})\rangle - \frac{1}{\sqrt{2}}|\text{Cube}_2(j,\vec{z},\vec{a})\rangle. \tag{7.91}$$

We prove

Lemma 23. *The Hamiltonian $H(G_2, G_X oc, n)$ has nullspace S_2 spanned by the states*

$$|C(j,\vec{z},\vec{a})\rangle$$

for $j \in [M]$ and $\vec{z}, \vec{a} \in \{0,1\}^n$. Its smallest nonzero eigenvalue is

$$\gamma(H(G_2, G_X oc, n)) \geq \frac{\mathcal{K}_0}{35000n}$$

where $\mathcal{K}_0 \in (0,1]$ is the absolute constant from Lemma 20.

Proof. Recall from the previous section that $H_1|_{S_1}$ is block diagonal in the basis (7.83), with a block for each $j \in [M]$ and $\vec{z}, \vec{a} \in \{0,1\}^n$. That is to say, $\langle k, \vec{c}, \text{In}(\vec{x}), \vec{b}|H_1|j, \vec{d}, \text{In}(\vec{z}), \vec{a}\rangle$ is zero unless $\vec{a} = \vec{b}$, $k = j$, and $\vec{z} = \vec{x}$. Equation (7.85) gives the nonzero matrix elements within a given block, which we use to compute the frustration-free ground states of $H_1|_{S_1}$.

Looking at equation (7.85), we see that the matrix for each block can be written as a sum of n commuting matrices: $\frac{n-1}{64}$ times the identity matrix (case 1 in equation (7.85)), $n-2$ terms that each flip a single bit $i \notin \{1, s(j)\}$ of $\vec{d}$ (case 2), and a term that changes the value of the "special" components $d_1 = d_{s(j)} \in \{0,1,2\}$ (case 3). Thus

$$\langle j, \vec{c}, \text{In}(\vec{z}), \vec{a}|H_1|j, \vec{d}, \text{In}(\vec{z}), \vec{a}\rangle = \langle j, \vec{c}, \text{In}(\vec{z}), \vec{a}|\frac{1}{64}(n-1) + \frac{1}{64}\sum_{i \in [n]\setminus\{1,s(j)\}} H_{\text{flip},i} + \frac{1}{64}H_{\text{special},j}|j, \vec{d}, \text{In}(\vec{z}), \vec{a}\rangle$$

where

$$\langle j, \vec{c}, \text{In}(\vec{z}), \vec{a}|H_{\text{flip},i}|j, \vec{d}, \text{In}(\vec{z}), \vec{a}\rangle = \delta_{c_i, d_i \oplus 1} \prod_{r \in [n]\setminus\{i\}} \delta_{c_r, d_r}$$

and

$$\langle j, \vec{c}, \text{In}(\vec{z}), \vec{a}|H_{\text{special},j}|j, \vec{d}, \text{In}(\vec{z}), \vec{a}\rangle = \begin{cases} \frac{1}{\sqrt{2}} & (c_1, d_1) \in \{(2,0),(0,2),(1,2),(2,1)\} \\ & \text{and } d_r = c_r \text{ for } r \in [n] \setminus \{1, s(j)\} \\ 0 & \text{otherwise.} \end{cases}$$

Note that these n matrices are mutually commuting, each eigenvalue of $H_{\text{flip},i}$ is ± 1, and each eigenvalue of $H_{\text{special},j}$ is equal to one of the eigenvalues of the matrix

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix},$$

which are $\{-1, 0, 1\}$. Thus we see that the eigenvalues of $H_1|_{S_1}$ within a block for some $j \in [M]$ and $\vec{z}, \vec{a} \in \{0,1\}^n$ are

$$\frac{1}{64}\left(n - 1 + \sum_{i \notin \{1,s(j)\}} y_i + w\right) \tag{7.92}$$

where $y_i \in \pm 1$ for each $i \in [n] \setminus \{1, s(j)\}$ and $w \in \{-1, 0, 1\}$. In particular, the smallest eigenvalue within the block is zero (corresponding to $y_i = w = -1$). The corresponding eigenspace is spanned by the simultaneous -1 eigenvectors of each $H_{\mathrm{flip},i}$ for $i \in [n] \setminus \{1, s(j)\}$ and $H_{\mathrm{special},j}$. The space of simultaneous -1 eigenvectors of $H_{\mathrm{flip},i}$ for $i \in [n] \setminus \{1, s(j)\}$ within the block is spanned by $\{|\mathrm{Cube}_0(j, \vec{z}, \vec{a})\rangle, |\mathrm{Cube}_1(j, \vec{z}, \vec{a})\rangle, |\mathrm{Cube}_2(j, \vec{z}, \vec{a})\rangle\}$. The state $|C(j, \vec{z}, \vec{a})\rangle$ is the unique superposition of these states that is a -1 eigenvector of $H_{\mathrm{special},j}$. Hence, for each block we obtain a unique state $|C(j, \vec{z}, \vec{a})\rangle$ in the space S_2. Ranging over all blocks $j \in [M]$ and $\vec{z}, \vec{a} \in \{0,1\}^n$, we get the basis described in the Lemma.

The smallest nonzero eigenvalue within each block is $\frac{1}{64}$ (corresponding to $y_i = -1$ and $w = 0$ in equation (7.92)), so

$$\gamma(H_1|_{S_1}) = \frac{1}{64}. \tag{7.93}$$

To get the stated lower bound, we use Lemma **??** with $H(G_2, G_X oc, n) = H_A + H_B$ where

$$H_A = H(G_1, G_X oc, n) \qquad H_B = H_1|_{\mathcal{I}(G_2, G_X oc, n)}$$

(as in equation (7.60)), along with the bounds

$$\gamma(H_A) \geq \frac{\mathcal{K}_0}{256} \qquad \gamma(H_B|_{S_1}) = \gamma(H_1|_{S_1}) = \frac{1}{64} \qquad \|H_B\| \leq \|H_1\| \leq n\,\|h_1\| = 2n$$

from Lemma 22, equations (7.64) and (7.93), and the fact that $\|h_1\| = 2$ from (7.21). This gives

$$\gamma(H(G_2, G_X oc, n)) \geq \frac{\mathcal{K}_0}{64\mathcal{K}_0 + 256 + 2n \cdot 64 \cdot 256} \geq \frac{\mathcal{K}_0}{35000n}$$

where we used the facts that $\mathcal{K}_0 \leq 1$ and $n \geq 1$. □

For each $\vec{z}, \vec{a} \in \{0,1\}^n$ define the uniform superposition

$$|\mathcal{H}(\vec{z}, \vec{a})\rangle = \frac{1}{\sqrt{M}} \sum_{j=1}^{M} |C\,(j, \vec{z}, \vec{a})\rangle.$$

that encodes (somewhat elaborately) the history of the computation that consists of applying either $U_{\mathcal{C}_X}$ or $U^*_{\mathcal{C}_X}$ to the state $|\vec{z}\rangle$. The first bit of $\vec{a}$ determines whether the circuit $\mathcal{C}_X$ or its complex conjugate is applied.

Lemma 24. *The Hamiltonian $H(G_3, G_X oc, n)$ has nullspace S_3 spanned by the states*

$$|\mathcal{H}(\vec{z}, \vec{a})\rangle$$

for $\vec{z}, \vec{a} \in \{0,1\}^n$. Its smallest nonzero eigenvalue is

$$\gamma(H(G_3, G_X oc, n)) \geq \frac{\mathcal{K}_0}{10^7 n^2 M^2}$$

where $\mathcal{K}_0 \in (0, 1]$ is the absolute constant from Lemma 20.

Proof. Recall that

$$H(G_3, G_X oc, n) = H(G_2, G_X oc, n) + H_2|_{\mathcal{I}(G_3, G_X oc, n)}$$

with both terms on the right-hand side positive semidefinite. To solve for the nullspace of $H(G_3, G_X oc, n)$, it suffices to restrict our attention to the space

$$S_2 = \mathrm{span}\{|C(j, \vec{z}, \vec{a})\rangle : j \in [M],\ \vec{z}, \vec{a} \in \{0,1\}^n\} \tag{7.94}$$

of states in the nullspace of $H(G_2, G_X oc, n)$. We begin by computing the matrix elements of H_2 in the basis for S_2 given above. We use equations (7.86) and (7.91) to compute the diagonal matrix elements:

$$\langle C\,(j, \vec{z}, \vec{a})\,|H_2|C\,(j, \vec{z}, \vec{a})\rangle = \frac{1}{4}\langle \mathrm{Cube}_0(j, \vec{z}, \vec{a})|H_2|\mathrm{Cube}_0(j, \vec{z}, \vec{a})\rangle + \frac{1}{4}\langle \mathrm{Cube}_1(j, \vec{z}, \vec{a}))|H_2|\mathrm{Cube}_1(j, \vec{z}, \vec{a})\rangle \tag{7.95}$$

$$+ \frac{1}{2}\langle \mathrm{Cube}_2(j, \vec{z}, \vec{a})|H_2|\mathrm{Cube}_2(j, \vec{z}, \vec{a})\rangle \tag{7.96}$$

$$= \begin{cases} 0 + \frac{1}{256} + \frac{1}{256} & j = 1 \\ \frac{1}{256} + \frac{1}{256} + \frac{1}{128} & j \in \{2, \ldots, M-1\} \\ \frac{1}{256} + 0 + \frac{1}{256} & j = M \end{cases} \tag{7.97}$$

$$= \begin{cases} \frac{1}{128} & j \in \{1, M\} \\ \frac{1}{64} & j \in \{2, \ldots, M-1\}. \end{cases} \tag{7.98}$$

In the second line we used equation (7.87). Looking at equation (7.86), we see that the only nonzero off-diagonal matrix elements of H_2 in this basis are of the form

$$\langle C(j-1, \vec{z}, \vec{a})|H_2|C(j, \vec{z}, \vec{a})\rangle \quad \text{or} \quad \langle C(j, \vec{z}, \vec{a})|H_2|C(j-1, \vec{z}, \vec{a})\rangle = \langle C(j-1, \vec{z}, \vec{a})|H_2|C(j, \vec{z}, \vec{a})\rangle^*$$

for $j \in \{2, \ldots, M\}$, $\vec{z}, \vec{a} \in \{0,1\}^n$. To compute these matrix elements we first use equation (7.88) to evaluate

$$\langle \mathrm{Cube}_w(j-1, \vec{z}, \vec{a})|H_2|\mathrm{Cube}_v(j, \vec{z}, \vec{a})\rangle$$

for $v, w \in \{0, 1, 2\}$ and $j \in \{2, \ldots, M\}$. For example, using the second case of equation (7.88), we get

$$\begin{aligned}\langle \mathrm{Cube}_1\,(j-1, \vec{z}, \vec{a})|H_2|\mathrm{Cube}_0\,(j, \vec{z}, \vec{a})\rangle &= \frac{1}{2^{n-2}} \sum_{\vec{d} \in \mathcal{D}_0^j} \sum_{\vec{c} \in \mathcal{D}_1^{j-1}} (-1)^{\sum_{i\in[n]}(c_i+d_i)} \langle j-1, \vec{c}, \mathrm{In}(\vec{z}), \vec{a}|H_2|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle \\ &= \frac{1}{2^{n-2}} \sum_{\vec{d} \in \mathcal{D}_0^j : d_{s(j-1)}=1} (-1) \cdot \frac{1}{64} = -\frac{1}{128}.\end{aligned}$$

To go from the first to the second line we used the fact that, for each $\vec{d} \in \mathcal{D}_0^j$ with $d_{s(j-1)} = 1$, there is one $\vec{c} \in \mathcal{D}_1^{j-1}$ for which $\langle j-1, \vec{c}, \mathrm{In}(\vec{z}), \vec{a}|H_2|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle = \frac{1}{64}$ (with all other such matrix elements equal to zero). This $\vec{c}$ satisfies $c_1 = c_{s(j-1)} = 1$ and $c_{s(j)} = 0$, with all other bits equal to those of $\vec{d}$, so

$$(-1)^{\sum_{i=1}^{n}(c_i+d_i)} = (-1)^{c_1+c_{s(j)}+c_{s(j-1)}+d_1+d_{s(j)}+d_{s(j-1)}} = -1$$

for each nonzero term in the sum.

We perform a similar calculation using cases 1, 3, and 4 in equation (7.88) to obtain

$$\langle \mathrm{Cube}_w(j-1,\vec{z},\vec{a})|H_2|\mathrm{Cube}_v(j,\vec{z},\vec{a})\rangle = \begin{cases} -\frac{1}{128} & (w,v)=(1,0) \\ \frac{1}{128\sqrt{2}} & (w,v)\in\{(2,0),(1,2)\} \\ -\frac{1}{256} & (w,v)=(2,2) \\ 0 & \text{otherwise.} \end{cases}$$

Hence

$$\begin{aligned}
&\langle C\left(j-1,\vec{z},\vec{a}\right)|H_2|C\left(j,\vec{z},\vec{a}\right)\rangle \\
&\quad= \frac{1}{4}\langle \mathrm{Cube}_1\left(j-1,\vec{z},\vec{a}\right)|H_2|\mathrm{Cube}_0\left(j,\vec{z},\vec{a}\right)\rangle - \frac{1}{2\sqrt{2}}\langle \mathrm{Cube}_2\left(j-1,\vec{z},\vec{a}\right)|H_2|\mathrm{Cube}_0\left(j,\vec{z},\vec{a}\right)\rangle \\
&\qquad+ \frac{1}{2}\langle \mathrm{Cube}_2\left(j-1,\vec{z},\vec{a}\right)|H_2|\mathrm{Cube}_2\left(j,\vec{z},\vec{a}\right)\rangle - \frac{1}{2\sqrt{2}}\langle \mathrm{Cube}_1\left(j-1,\vec{z},\vec{a}\right)|H_2|\mathrm{Cube}_2\left(j,\vec{z},\vec{a}\right)\rangle \\
&\quad= -\frac{1}{128}.
\end{aligned}$$

Combining this with equation (7.98), we see that $H_2|_{S_2}$ is block diagonal in the basis (7.94), with a block for each pair of n-bit strings $\vec{z},\vec{a}\in\{0,1\}^n$. Each of the 2^{2n} blocks is equal to the $M\times M$ matrix

$$\frac{1}{128}\begin{pmatrix} 1 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \ddots & \vdots \\ 0 & 0 & -1 & \ddots & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & 2 & -1 \\ 0 & 0 & \cdots & 0 & -1 & 1 \end{pmatrix}.$$

This matrix is just $\frac{1}{128}$ times the Laplacian of a path of length M, whose spectrum is well known. In particular, it has a unique eigenvector with eigenvalue zero (the all-ones vector) and its eigenvalue gap is $2(1-\cos(\frac{\pi}{M}))\geq\frac{4}{M^2}$. Thus for each of the 2^{2n} blocks there is an eigenvector of $H_2|_{S_2}$ with eigenvalue 0, equal to the uniform superposition $|\mathcal{H}(\vec{z},\vec{a})\rangle$ over the M states in the block. Furthermore, the smallest nonzero eigenvalue within each block is at least $\frac{1}{32M^2}$. Hence

$$\gamma(H_2|_{S_2})\geq\frac{1}{32M^2}. \tag{7.99}$$

To get the stated lower bound on $\gamma(H(G_3,G_Xoc,n))$, we apply Lemma **??** with

$$H_A = H(G_2,G_Xoc,n) \qquad H_B = H_2|_{\mathcal{I}(G_3,G_Xoc,n)}$$

and

$$\gamma(H_A) \geq \frac{\mathcal{K}_0}{35000n} \qquad \gamma(H_B|_{S_2}) = \gamma(H_2|_{S_2}) \geq \frac{1}{32M^2} \qquad \|H_B\| \leq \|H_2\| \leq n\|h_2\| = 2n \tag{7.100}$$

from Lemma 23, equation (7.99), and the fact that $\|h_2\| = 2$ from (7.21). This gives

$$\begin{aligned}\gamma(H(G_3, G_X oc, n)) &\geq \frac{\mathcal{K}_0}{32M^2\mathcal{K}_0 + 35000n + 2n(35000n)(32M^2)} \\ &\geq \frac{\mathcal{K}_0}{M^2n^2(32 + 35000 + 70000 \cdot 32)} \geq \frac{\mathcal{K}_0}{10^7 M^2 n^2}.\end{aligned}$$

□

Lemma 25. *The nullspace S_4 of $H(G_4, G_X oc, n)$ is spanned by the states*

$$|\mathcal{H}(\vec{z}, \vec{a})\rangle \quad \text{where} \quad \vec{z} = z_1 z_2 \dots z_{n_{in}} \underbrace{00\dots0}_{n-n_{in}} \tag{7.101}$$

for $\vec{a} \in \{0,1\}^n$ and $z_1, \dots, z_{n_{in}} \in \{0,1\}$. Its smallest nonzero eigenvalue satisfies

$$\gamma(H(G_4, G_X oc, n)) \geq \frac{\mathcal{K}_0}{10^{10} M^3 n^3}$$

where $\mathcal{K}_0 \in (0,1]$ is the absolute constant from Lemma 20.

Proof. Using equation (7.89), we find

$$\begin{aligned}\langle C(k, \vec{x}, \vec{b})|H_{\mathrm{in},i}|C(j, \vec{z}, \vec{a})\rangle &= \delta_{k,j}\delta_{\vec{x},\vec{z}}\delta_{\vec{a},\vec{b}}\bigg(\frac{1}{4}\langle \mathrm{Cube}_0(j, \vec{z}, \vec{a})|H_{\mathrm{in},i}|\mathrm{Cube}_0(j, \vec{z}, \vec{a})\rangle \\ &\quad + \frac{1}{4}\langle \mathrm{Cube}_1(j, \vec{z}, \vec{a})|H_{\mathrm{in},i}|\mathrm{Cube}_1(j, \vec{z}, \vec{a})\rangle \\ &\quad + \frac{1}{2}\langle \mathrm{Cube}_2(j, \vec{z}, \vec{a})|H_{\mathrm{in},i}|\mathrm{Cube}_2(j, \vec{z}, \vec{a})\rangle\bigg) \\ &= \delta_{k,j}\delta_{\vec{x},\vec{z}}\delta_{\vec{a},\vec{b}}\left(\frac{1}{64}\delta_{z_i,1}\right)\begin{cases}\frac{1}{4}\cdot\frac{1}{2} + \frac{1}{4}\cdot\frac{1}{2} + \frac{1}{2}\cdot\frac{1}{2} & j < j_{\min,i} \\ \frac{1}{4} + 0 + 0 & j = j_{\min,i} \\ 0 + 0 + 0 & j > j_{\min,i}\end{cases}\end{aligned}$$

for each $i \in \{n_{\mathrm{in}} + 1, \dots, n\}$. Hence

$$\langle \mathcal{H}(\vec{x}, \vec{b})| \sum_{i=n_{\mathrm{in}}+1}^{n} H_{\mathrm{in},i} |\mathcal{H}(\vec{z}, \vec{a})\rangle = \frac{1}{M}\delta_{\vec{x},\vec{z}}\delta_{\vec{a},\vec{b}} \sum_{i=n_{\mathrm{in}}+1}^{n} \frac{1}{64}\left(\frac{j_{\min,i} - 1}{2} + \frac{1}{4}\right)\delta_{z_i,1}.$$

Therefore

$$\sum_{i=n_{\mathrm{in}}+1}^{n} H_{\mathrm{in},i}\big|_{S_3}$$

is diagonal in the basis $\{|\mathcal{H}(\vec{z}, \vec{a})\rangle : \vec{z}, \vec{a} \in \{0,1\}^n\}$. The zero eigenvectors are given by equation (7.101), and the smallest nonzero eigenvalue is

$$\gamma\left(\sum_{i=n_{\mathrm{in}}+1}^{n} H_{\mathrm{in},i}\big|_{S_3}\right) \geq \frac{1}{256M}. \tag{7.102}$$

since $j_{\min,i} \geq 1$. To get the stated lower bound we now apply Lemma **??** with

$$H_A = H(G_3, G_X oc, n) \qquad H_B = \sum_{i=n_{\text{in}}+1}^{n} H_{\text{in},i}\big|_{\mathcal{I}(G_4, G_X oc, n)}$$

and

$$\gamma(H_A) \geq \frac{\mathcal{K}_0}{10^7 M^2 n^2} \qquad \gamma(H_B|_{S_3}) \geq \frac{1}{256M} \qquad \|H_B\| \leq n \left\| \sum_{i=n_{\text{in}}+1}^{n} h_{\text{in},i} \right\| = n$$

where we used Lemma 24, equation (7.102), and the fact that $\left\|\sum_{i=n_{\text{in}}+1}^{n} h_{\text{in},i}\right\| = 1$ (from equation (7.20). This gives

$$\begin{aligned}
\gamma\left(H(G_4, G_X oc, n)\right) &\geq \frac{\mathcal{K}_0}{256M\mathcal{K}_0 + 10^7 n^2 M^2 + n(256M)(10^7 n^2 M^2)} \\
&\geq \frac{\mathcal{K}_0}{(M^3 n^3)(256 + 10^7 + 256 \cdot 10^7)} \geq \frac{\mathcal{K}_0}{10^{10} M^3 n^3}.
\end{aligned}$$

□

7.3.4 The occupancy constraints lemma

7.3.4.1 Definitions and notation

In this Section we establish notation and we describe how the gate graph $G^{\square}$ is constructed from G and G^{occ}. We also define two related gate graphs $G^{\triangle}$ and $G^{\diamond}$ that we use in our analysis.

Let us first fix notation for the gate graph G and the occupancy constraints graph G^{occ}. Write the adjacency matrix of G as (see equation (7.17))

$$A(G) = \sum_{q=1}^{R} |q\rangle\langle q| \otimes A(g_0) + h_{\mathcal{E}^G} + h_{\mathcal{S}^G}$$

where $h_{\mathcal{E}^G}$ and $h_{\mathcal{S}^G}$ are determined (through equations (7.19) and (7.18)) by the sets $\mathcal{E}^G$ and $\mathcal{S}^G$ of edges and self-loops in the gate diagram for G, and where g_0 is the 128-vertex graph from Figure **??**. Recall that the occupancy constraints graph G^{occ} is a simple graph with vertices labeled $q \in [R]$, one for each diagram element in G. We write $E(G^{\text{occ}}) \subseteq \binom{[R]}{2} = \{\{x, y\} \colon x, y \in [R],\, x \neq y\}$ for the edge set of G^{occ}.

Definition of $G^{\square}$

To ensure that the ground space has the appropriate form, the construction of $G^{\square}$ is slightly different depending on whether R is even or odd. The following description handles both cases.

1. Replace each diagram element $q \in [R]$ in the gate diagram for G as shown in Figure **??**, with diagram elements labeled $q_{\text{in}}, q_{\text{out}}$ and $d(q, s)$ where $q, s \in [R]$ and $q \neq s$ if R is

even. Each node (q,z,t) in the gate diagram for G is mapped to a new node $\mathrm{new}(q,z,t)$ as shown by the black and grey arrows, i.e.,

$$\mathrm{new}(q,z,t)=\begin{cases}(q_{\mathrm{in}},z,t) & \text{if } (q,z,t) \text{ is an input node}\\ (q_{\mathrm{out}},z,t) & \text{if } (q,z,t) \text{ is an output node.}\end{cases} \tag{7.103}$$

Edges and self-loops in the gate diagram for G are replaced by edges and self-loops between the corresponding nodes in the modified diagram.

2. For each edge $\{q_1,q_2\}\in E(G^{\mathrm{occ}})$ in the occupancy constraints graph we add four diagram elements of the type shown in Figure **??** (i.e., diagram elements corresponding to the identity). We refer to these diagram elements by labels $e_{ij}(q_1,q_2)$ with $i,j\in\{0,1\}$. For these diagram elements the labeling function is symmetric, i.e., $e_{ij}(q_1,q_2)=e_{ji}(q_2,q_1)$ whenever $\{q_1,q_2\}\in E(G^{\mathrm{occ}})$.

3. For each non-edge $\{q_1,q_2\}\notin E(G^{\mathrm{occ}})$ with $q_1,q_2\in[R]$ and $q_1\neq q_2$ we add 8 diagram elements of the type shown in Figure **??**. We refer to these diagram elements as $e_{ij}(q_1,q_2)$ and $e_{ij}(q_2,q_1)$ with $i,j\in\{0,1\}$; when $\{q_1,q_2\}\notin E(G^{\mathrm{occ}})$ the labeling function is not symmetric, i.e., $e_{ij}(q_1,q_2)\neq e_{ji}(q_2,q_1)$. If R is odd we also add $4R$ diagram elements labeled $e_{ij}(q,q)$ with $i,j\in\{0,1\}$ and $q\in[R]$.

4. Finally, we add edges and self-loops to the gate diagram as shown in Figure **??**. This gives the gate diagram for $G^{\square}$.

The set of diagram elements in the gate graph for $G^{\square}$ is indexed by

$$L^{\square}=Q_{\mathrm{in}}\cup D\cup E_{\mathrm{edges}}\cup E_{\text{non-edges}}\cup Q_{\mathrm{out}} \tag{7.104}$$

where

$$\begin{aligned}
Q_{\mathrm{in}}&=\{q_{\mathrm{in}}:q\in[R]\} && (7.105)\\
D&=\{d(q,s):\ q,s\in[R] \text{ and } q\neq s \text{ if } R \text{ is even}\} && (7.106)\\
E_{\mathrm{edges}}&=\{e_{ij}(q,s):\ i,j\in\{0,1\},\ \{q,s\}\in E(G^{\mathrm{occ}}) \text{ and } q<s\}\\
E_{\text{non-edges}}&=\{e_{ij}(q,s):\ i,j\in\{0,1\},\ \{q,s\}\notin E(G^{\mathrm{occ}}) \text{ and } q\neq s \text{ if } R \text{ is even}\}\\
Q_{\mathrm{out}}&=\{q_{\mathrm{out}}:q\in[R]\}\,. && (7.107)
\end{aligned}$$

The total number of diagram elements in $G^{\square}$ is

$$\begin{aligned}
|L^{\square}|&=|Q_{\mathrm{in}}|+|D|+|E_{\mathrm{edges}}|+|E_{\text{non-edges}}|+|Q_{\mathrm{out}}|\\
&=\begin{cases}R+R^2+4|E(G^{\mathrm{occ}})|+4\left(R^2-2|E(G^{\mathrm{occ}})|\right)+R & R \text{ odd}\\ R+R\,(R-1)+4|E(G^{\mathrm{occ}})|+4\left(R(R-1)-2|E(G^{\mathrm{occ}})|\right)+R & R \text{ even}\end{cases}\\
&=\begin{cases}5R^2+2R-4|E(G^{\mathrm{occ}})| & R \text{ odd}\\ 5R^2-3R-4|E(G^{\mathrm{occ}})| & R \text{ even.}\end{cases}
\end{aligned}$$

In both cases this is upper bounded by $7R^2$ as claimed in the statement of the Lemma. Write

$$A(G^{\square}) = \sum_{l\in L^{\square}} |l\rangle\langle l| \otimes A(g_0) + h_{\mathcal{S}^{\square}} + h_{\mathcal{E}^{\square}} \tag{7.108}$$

where $\mathcal{S}^{\square}$ and $\mathcal{E}^{\square}$ are the sets of self-loops and edges in the gate diagram for $G^{\square}$.

We now focus on the input nodes of diagram elements in Q_{in} and the output nodes of the diagram elements in Q_{out}. These are the nodes indicated by the black and grey arrows in Figure **??**. Write $\mathcal{E}^0 \subset \mathcal{E}^{\square}$ and $\mathcal{S}^0 \subset \mathcal{S}^{\square}$ for the sets of edges and self-loops that are incident on these nodes in the gate diagram for $G^{\square}$. Note that the sets $\mathcal{E}^0$ and $\mathcal{S}^0$ are in one-to-one correspondence with (respectively) the sets $\mathcal{E}^G$ and $\mathcal{S}^G$ of edges and self-loops in the gate diagram for G. The other edges and self-loops in $G^{\square}$ do not depend on the sets of edges and self-loops in G. Writing

$$\mathcal{S}^{\triangle} = \mathcal{S}^{\square} \setminus S^0 \qquad \mathcal{E}^{\triangle} = \mathcal{E}^{\square} \setminus \mathcal{E}^0,$$

we have

$$h_{\mathcal{S}^{\square}} = h_{\mathcal{S}^0} + h_{\mathcal{S}^{\triangle}} \qquad h_{\mathcal{E}^{\square}} = h_{\mathcal{E}^0} + h_{\mathcal{E}^{\triangle}}. \tag{7.109}$$

Definition of $G^{\triangle}$

The gate diagram for $G^{\triangle}$ is obtained from that of $G^{\square}$ by removing all edges and self-loops attached to the input nodes of the diagram elements in Q_{in} and the output nodes of the diagram elements in Q_{out}. Its adjacency matrix is

$$A(G^{\triangle}) = \sum_{l\in L^{\square}} |l\rangle\langle l| \otimes A(g_0) + h_{\mathcal{S}^{\triangle}} + h_{\mathcal{E}^{\triangle}}. \tag{7.110}$$

Note that $G^{\triangle} = G^{\square}$ whenever the gate diagram for G contains no edges or self-loops.

Definition of $G^{\diamondsuit}$

We also define a gate graph $G^{\diamondsuit}$ with gate diagram obtained from that of $G^{\triangle}$ by removing all edges (but leaving the self-loops). Note that $G^{\diamondsuit}$ has a component for each diagram element $l \in L^{\square}$. The components corresponding to diagram elements without a self-loop (those with $l \in L^{\square} \setminus E_{\text{non-edges}}$) have adjacency matrix $A(g_0)$; those with a self-loop ($l \in E_{\text{non-edges}}$) have adjacency matrix $A(g_0) + |1,1\rangle\langle 1,1| \otimes \mathbb{I}$, so

$$A(G^{\diamondsuit}) = \sum_{l\in L^{\square}} |l\rangle\langle l| \otimes A(g_0) + h_{\mathcal{S}^{\triangle}} \tag{7.111}$$

$$= \sum_{l\in L^{\square}\setminus E_{\text{non-edges}}} |l\rangle\langle l| \otimes A(g_0) + \sum_{l\in E_{\text{non-edges}}} |l\rangle\langle l| \otimes \left(A(g_0) + |1,1\rangle\langle 1,1| \otimes \mathbb{I}\right). \tag{7.112}$$

Example

We provide an example of this construction in Figure **??** (which shows a gate graph and an occupancy constraints graph) and Figure **??** (which describes the derived gate graphs $G^{\square}$, $G^{\triangle}$, and $G^{\diamondsuit}$).

7.3.5 The gate graph $G^{\diamondsuit}$

We now solve for the e_1-energy ground states of the adjacency matrix $A(G^{\diamondsuit})$. Write g_1 for the graph with adjacency matrix

$$A(g_1) = A(g_0) + |1,1\rangle\langle 1,1| \otimes \mathbb{I}$$

(i.e., g_0 with 8 self-loops added), so (recalling equation (7.112)) each component of $G^{\diamondsuit}$ is either g_0 or g_1. Recall from Section **??** that $A(g_0)$ has four orthonormal e_1-energy ground states $|\psi_{z,a}\rangle$ with $z, a \in \{0,1\}$. It is also not hard to verify that the e_1-energy ground space of $A(g_1)$ is spanned by two of these states $|\psi_{0,a}\rangle$ for $a \in \{0,1\}$. Now letting $|\psi_{z,a}^l\rangle = |l\rangle|\psi_{z,a}\rangle$, we choose a basis $\mathcal{W}$ for the e_1-energy ground space of $A(G^{\diamondsuit})$ where each basis vector is supported on one of the components:

$$\mathcal{W} = \big\{|\psi_{z,a}^l\rangle : z, a \in \{0,1\},\, l \in L^{\square} \setminus E_{\text{non-edges}}\big\} \cup \big\{|\psi_{0,a}^l\rangle : a \in \{0,1\},\, l \in E_{\text{non-edges}}\big\}. \quad (7.113)$$

The eigenvalue gap of $A(G^{\diamondsuit})$ is equal to that of either $A(g_0)$ or $A(g_1)$. Since g_0 and g_1 are specific 128-vertex graphs we can calculate their eigenvalue gaps using a computer; we get $\gamma(A(g_0) - e_1) = 0.7785\ldots$ and $\gamma(A(g_1) - e_1) = 0.0832\ldots$. Hence

$$\gamma(A(G^{\diamondsuit}) - e_1) \geq 0.0832\ldots > \frac{1}{13}. \quad (7.114)$$

The ground space of $A(G^{\diamondsuit})$ has dimension

$$\begin{aligned} |\mathcal{W}| = 4\left|L^{\square}\right| - 2\left|E_{\text{non-edges}}\right| &= \begin{cases} 4\left(5R^2 + 2R - 4|E(G^{\text{occ}})|\right) - 2\left(4R^2 - 8|E(G^{\text{occ}})|\right) & R \text{ odd} \\ 4\left(5R^2 - 3R - 4|E(G^{\text{occ}})|\right) - 2\left(4R(R-1) - 8|E(G^{\text{occ}})|\right) & R \text{ even} \end{cases} \\ &= \begin{cases} 12R^2 + 8R & R \text{ odd} \\ 12R^2 - 4R & R \text{ even.} \end{cases} \end{aligned} \quad (7.115)$$

We now consider the N-particle Hamiltonian $H(G^{\diamondsuit}, N)$ and characterize its nullspace.

Lemma 26. *The nullspace of $H(G^{\diamondsuit}, N)$ is*

$$\mathcal{I}_{\diamondsuit} = \text{span}\{\text{Sym}(|\psi_{z_1,a_1}^{q_1}\rangle|\psi_{z_2,a_2}^{q_2}\rangle \ldots |\psi_{z_N,a_N}^{q_N}\rangle) : |\psi_{z_i,a_i}^{q_i}\rangle \in \mathcal{W} \text{ and } q_i \neq q_j \text{ for all distinct } i,j \in [N]\}$$

where $\mathcal{W}$ is given in equation (7.113). The smallest nonzero eigenvalue satisfies $\gamma(H(G^{\diamondsuit}, N)) > \frac{1}{300}$.

Proof. For the first part of the proof we use the fact that the basis vectors $|\psi_{z,a}^l\rangle \in \mathcal{W}$ span the e_1-eigenspace of the component $G_l^{\diamondsuit}$ of $G^{\diamondsuit}$ corresponding to the diagram element $l \in L^{\square}$, i.e., the nullspace of $H(G_l^{\diamondsuit}, 1)$. Furthermore, no component of $G^{\diamondsuit}$ supports a two-particle frustration-free state, i.e., $\lambda_2^1(g_0) > 0$ and $\lambda_2^1(g_1) > 0$ (by Lemma 13). Now applying Lemma 12 we see that $\mathcal{I}_{\diamondsuit}$ is the nullspace of $H(G^{\diamondsuit}, N)$. We also see that the smallest nonzero eigenvalue $\gamma(H(G^{\diamondsuit}, N))$ is either $\lambda_2^1(g_0)$, $\lambda_2^1(g_1)$, $\gamma(H(g_0, 1))$, or $\gamma(H(g_1, 1))$. These constants can be calculated numerically using a computer; they are $\lambda_2^1(g_0) = 0.0035\ldots$, $\lambda_2^1(g_1) = 0.0185\ldots$, $\gamma(H(g_0, 1)) = 0.7785\ldots$, and $\gamma(H(g_1, 1)) = 0.0832\ldots$. Hence

$$\gamma(H(G^{\diamondsuit}, N)) \geq \min\{\lambda_2^1(g_0), \lambda_2^1(g_1), \gamma(H(g_0, 1)), \gamma(H(g_1, 1))\} > \frac{1}{300}. \qquad \square$$

7.3.6 The adjacency matrix of the gate graph $G^{\triangle}$

We begin by solving for the e_1-energy ground space of the adjacency matrix $A(G^{\triangle})$. From equations (7.110) and (7.111) we have

$$A(G^{\triangle}) = A(G^{\diamondsuit}) + h_{\mathcal{E}^{\triangle}}. \tag{7.116}$$

Recall the e_1-energy ground space of $A(G^{\diamondsuit})$ is spanned by $\mathcal{W}$ from equation (7.113). Since $h_{\mathcal{E}^{\triangle}} \geq 0$ it follows that $A(G^{\triangle}) \geq e_1$. To solve for the e_1-energy groundpsace of $A(G^{\triangle})$ we construct superpositions of vectors from $\mathcal{W}$ that are in the nullspace of $h_{\mathcal{E}^{\triangle}}$. To this end we consider the restriction

$$h_{\mathcal{E}^{\triangle}}\big|_{\mathrm{span}(\mathcal{W})}. \tag{7.117}$$

We now show that it is block diagonal in the basis $\mathcal{W}$ and we compute its matrix elements.

First recall from equation (7.19) that

$$h_{\mathcal{E}^{\triangle}} = \sum_{\{(l,z,t),(l',z',t')\}\in\mathcal{E}^{\triangle}} \left(|l,z,t\rangle + |l',z',t'\rangle\right)\left(\langle l,z,t| + \langle l',z',t'|\right) \otimes \mathbb{I}. \tag{7.118}$$

The edges $\{(l,z,t),(l',z',t')\} \in \mathcal{E}^{\triangle}$ can be read off from Figure **??** and Figure **??**, respectively (referring back to Figure **??** for our convention regarding the labeling of nodes on a diagram element). The edges from Figure **??** are

$$\{(q_{\text{in}},z,t),(d(q,1),z,t')\},\{(d(q,2),z,t),(d(q,3),z,t')\},\ldots,\{(d(q,R),z,t),(q_{\text{out}},z,t')\} \tag{7.119}$$

with $q \in [R]$ and $(z,t,t') = (0,7,3)$ or $(1,5,1)$, and where $d(q,q)$ does not appear if R is even (i.e., $d(q,q-1)$ is followed by $d(q,q+1)$. The edges from Figure **??** are

$$\begin{aligned}&\{(d(q,s),0,1),(e_{00}(q,s),\alpha(q,s),1)\},\{(d(q,s),1,3),(e_{10}(q,s),\alpha(q,s),1)\},\\&\{(d(q,s),0,5),(e_{01}(q,s),\alpha(q,s),1)\},\{(d(q,s),1,7),(e_{11}(q,s),\alpha(q,s),1)\}\end{aligned} \tag{7.120}$$

with $q,s \in [R]$ and $q \neq s$ if R is even, and where

$$\alpha(q,s) = \begin{cases} 1 & q > s \text{ and } \{q,s\} \in E(G^{\text{occ}}) \\ 0 & \text{otherwise.}\end{cases}$$

The set $\mathcal{E}^{\triangle}$ consists of all edges (7.119) and (7.120).

We claim that (7.117) is block diagonal with a block $\mathcal{W}_{(z,a,q)} \subseteq \mathcal{W}$ of size

$$\left|\mathcal{W}_{(z,a,q)}\right| = \begin{cases} 3R+2 & R \text{ odd} \\ 3R-1 & R \text{ even}\end{cases}$$

for each for each triple (z,a,q) with $z,a \in \{0,1\}$ and $q \in [R]$. Using equation (7.115) we confirm that $|\mathcal{W}| = 4R\left|\mathcal{W}_{(z,a,q)}\right|$, so this accounts for all basis vectors in $\mathcal{W}$. The subset of basis vectors for a given block is

$$\begin{aligned}\mathcal{W}_{(z,a,q)} = &\left\{|\psi_{z,a}^{q_{\text{in}}}\rangle, |\psi_{z,a}^{q_{\text{out}}}\rangle\right\} \cup \left\{|\psi_{z,a}^{d(q,s)}\rangle \colon s \in [R],\, s \neq q \text{ if } R \text{ even}\right\}\\ &\cup \left\{|\psi_{\alpha(q,s),a}^{e_{zx}(q,s)}\rangle \colon x \in \{0,1\},\, s \in [R],\, s \neq q \text{ if } R \text{ even}\right\}.\end{aligned} \tag{7.121}$$

Using equation (7.118) and the description of $\mathcal{E}^{\triangle}$ from (7.119) and (7.120), one can check by direct inspection that (7.117) only has nonzero matrix elements between basis vectors in $\mathcal{W}$ from the same block. We also compute the matrix elements between vectors from the same block. For example, if R is odd or if R is even and $q \neq 1$, there are edges $\{(q_{\text{in}}, 0, 7), (d(q, 1), 0, 3)\}, \{(q_{\text{in}}, 1, 5), (d(q, 1), 1, 1)\} \in \mathcal{E}^{\triangle}$. Using the fact that $|\psi^l_{z,a}\rangle = |l\rangle|\psi_{z,a}\rangle$ where $|\psi_{z,a}\rangle$ is given by (7.15) and (7.16), we compute the relevant matrix elements:

$$\begin{aligned}
&\langle\psi^{q_{\text{in}}}_{z,a}|h_{\mathcal{E}^{\triangle}}|\psi^{d(q,1)}_{z,a}\rangle \\
&\quad= \langle\psi^{q_{\text{in}}}_{z,a}|\left(\sum_{(z',t,t')\in\{(0,7,3),(1,5,1)\}} (|q_{\text{in}}, z', t\rangle + |d(q, 1), z', t'\rangle) (\langle q_{\text{in}}, z', t| + \langle d(q, 1), z', t'|) \otimes \mathbb{I}\right)|\psi^{d(q,1)}_{z,a}\rangle \\
&\quad= \sum_{(z',t,t')\in\{(0,7,3),(1,5,1)\}} \langle\psi_{z,a}| (|z', t\rangle\langle z', t'| \otimes \mathbb{I}) |\psi_{z,a}\rangle = \frac{1}{8}.
\end{aligned}$$

Continuing in this manner, we compute the principal submatrix of (7.117) corresponding to the set $\mathcal{W}_{(z,a,q)}$. This matrix is shown in Figure **??**. In the Figure each vertex is associated with a state in the block and the weight on a given edge is the matrix element between the two states associated with vertices joined by that edge. The diagonal matrix elements are described by the weights on the self-loops. The matrix described by Figure **??** is the same for each block.

For each triple (z, a, q) with $z, a \in \{0, 1\}$ and $q \in [R]$, define

$$|\phi^q_{z,a}\rangle = \begin{cases} \frac{1}{\sqrt{3R+2}} \left(|\psi^{q_{\text{in}}}_{z,a}\rangle + \sum_{j\in[R]} (-1)^j \left(|\psi^{d(q,j)}_{z,a}\rangle - |\psi^{e_{z0}(q,j)}_{\alpha(q,j),a}\rangle - |\psi^{e_{z1}(q,j)}_{\alpha(q,j),a}\rangle\right) + |\psi^{q_{\text{out}}}_{z,a}\rangle\right) & R \text{ odd} \\ \frac{1}{\sqrt{3R-1}} \left(|\psi^{q_{\text{in}}}_{z,a}\rangle + \left(\sum_{j<q} - \sum_{j>q}\right) (-1)^j \left(|\psi^{d(q,j)}_{z,a}\rangle - |\psi^{e_{z0}(q,j)}_{\alpha(q,j),a}\rangle - |\psi^{e_{z1}(q,j)}_{\alpha(q,j),a}\rangle\right) + |\psi^{q_{\text{out}}}_{z,a}\rangle\right) & R \text{ even.} \end{cases} \tag{7.122}$$

Next we show that these states span the ground space of $A(G^{\triangle})$. The choice to omit $d(q, q)$ for R even ensures that $|\psi^{q_{\text{in}}}_{z,a}\rangle$ and $|\psi^{q_{\text{out}}}_{z,a}\rangle$ have the same sign in these ground states.

Lemma 27. *An orthonormal basis for the e_1-energy ground space of $A(G^{\triangle})$ is given by the states*

$$\left\{|\phi^q_{z,a}\rangle : z, a \in \{0, 1\}, q \in [R]\right\}$$

defined by equation (7.122). The eigenvalue gap is bounded as

$$\gamma(A(G^{\triangle}) - e_1) > \frac{1}{(30R)^2}. \tag{7.123}$$

Proof. The e_1-energy ground space of $A(G^{\triangle})$ is equal to the nullspace of (7.117). Since this operator is block diagonal in the basis $\mathcal{W}$, we can solve for the eigenvectors in the nullspace of each block. Thus, to prove the first part of the Lemma, we analyze the $|\mathcal{W}_{(z,a,q)}| \times |\mathcal{W}_{(z,a,q)}|$ matrix described by Figure **??** and show that (7.122) is the unique vector in its nullspace. We first rewrite it in a slightly different basis obtained by multiplying some of the basis vectors by a phase of -1. Specifically, we use the basis

$$\left\{|\psi^{q_{\text{in}}}_{z,a}\rangle, -|\psi^{d(q,1)}_{z,a}\rangle, |\psi^{e_{z0}(q,1)}_{\alpha(q,1),a}\rangle, |\psi^{e_{z1}(q,1)}_{\alpha(q,1),a}\rangle, |\psi^{d(q,2)}_{z,a}\rangle, -|\psi^{e_{z0}(q,2)}_{\alpha(q,2),a}\rangle, -|\psi^{e_{z1}(q,2)}_{\alpha(q,2),a}\rangle, \ldots, |\psi^{q_{\text{out}}}_{z,a}\rangle\right\}$$

where the state associated with each vertex on one side of a bipartition of the graph is multiplied by -1; these are the phases appearing in equation (7.122). Changing to this basis replaces the weight $\frac{1}{8}$ on each edge in Figure ?? by $-\frac{1}{8}$ and does not change the weights on the self-loops. The resulting matrix is $\frac{1}{8}L_0$, where L_0 is the Laplacian matrix of the graph shown in Figure ??. Now we use the fact that the Laplacian of any connected graph has smallest eigenvalue zero, with a unique eigenvector equal to the all-ones vector. Hence for each block we get an eigenvector in the nullspace of (7.117)) given by (7.122). Ranging over all $z, a \in \{0, 1\}$ and $q \in [R]$ gives the claimed basis for the e_1-energy ground space of $A(G^{\triangle})$.

To prove the lower bound, we use the Nullspace Projection Lemma (Lemma ??) with

$$H_A = A(G^{\diamondsuit}) - e_1 \qquad H_B = h_{\mathcal{E}^{\triangle}}$$

and where $S = \operatorname{span}(\mathcal{W})$ is the nullspace of H_A as shown in Section 7.3.5. Since it is block diagonal in the basis $\mathcal{W}$, the smallest nonzero eigenvalue of (7.117) is equal to the smallest nonzero eigenvalue of one of its blocks. The matrix for each block is $\frac{1}{8}L_0$. Thus we can lower bound the smallest nonzero eigenvalue of $H_B|_S$ using standard bounds on the smallest nonzero eigenvalue of the Laplacian L of a graph G. In particular, Theorem 4.2 of reference [?] shows that

$$\gamma(L) \geq \frac{4}{|V(G)| \operatorname{diam}(G)} \geq \frac{4}{|V(G)|^2}$$

(where $\operatorname{diam}(G)$ is the diameter of G). Since the size of the graph in Figure ?? is either $3R - 1$ or $3R + 2$, we have

$$\gamma(H_B|_S) = \frac{1}{8}\gamma(L_0) \geq \frac{1}{8}\frac{4}{(3R+2)^2} \geq \frac{1}{32R^2}$$

since $R \geq 2$. Using this bound and the fact that $\gamma(H_A) > \frac{1}{13}$ (from equation (7.114)) and $\|H_B\| = 2$ (from equation (7.21)) and plugging into Lemma ?? gives

$$\gamma(A(G^{\triangle}) - e_1) \geq \frac{\frac{1}{13} \cdot \frac{1}{32R^2}}{\frac{1}{13} + \frac{1}{32R^2} + 2} \geq \frac{1}{(32 + 13 + 832)R^2} > \frac{1}{(30R)^2}. \qquad \square$$

7.3.7 The Hamiltonian $H(G^{\triangle}, N)$

We now consider the N-particle Hamiltonian $H(G^{\triangle}, N)$ and solve for its nullspace. We use the following fact about the subsets $\mathcal{W}_{(z,a,q)} \subset \mathcal{W}$ defined in equation (7.121).

Definition 12. We say $\mathcal{W}_{(z_1,a_1,q_1)}$ and $\mathcal{W}_{(z_2,a_2,q_2)}$ *overlap on a diagram element* if there exists $l \in L^{\square}$ such that $|\psi^l_{x_1,b_1}\rangle \in \mathcal{W}_{(z_1,a_1,q_1)}$ and $|\psi^l_{x_2,b_2}\rangle \in \mathcal{W}_{(z_2,a_2,q_2)}$ for some $x_1, x_2, b_1, b_2 \in \{0, 1\}$.

Fact 2 (Key property of $\mathcal{W}_{(z,a,q)}$)**.** *Sets $\mathcal{W}_{(z_1,a_1,q_1)}$ and $\mathcal{W}_{(z_2,a_2,q_2)}$ overlap on a diagram element if and only if $q_1 = q_2$ or $\{q_1, q_2\} \in E(G^{\text{occ}})$.*

This fact can be confirmed by direct inspection of the sets $\mathcal{W}_{(z,a,q)}$. If $q_1 = q_2 = q$ the diagram element l on which they overlap can be chosen to be $l = q_{\text{in}}$; if $q_1 \neq q_2$ and $\{q_1, q_2\} \in E(G^{\text{occ}})$ then $l = e_{z_1 z_2}(q_1, q_2) = e_{z_2 z_1}(q_2, q_1)$. Conversely, if $\{q_1, q_2\} \notin E(G^{\text{occ}})$ with $q_1 \neq q_2$, then there is no overlap.

We show that the nullspace $\mathcal{I}_\triangle$ of $H(G^\triangle, N)$ is

$$\mathcal{I}_\triangle = \operatorname{span}\{\mathrm{Sym}(|\phi^{q_1}_{z_1,a_1}\rangle|\phi^{q_2}_{z_2,a_2}\rangle \dots |\phi^{q_N}_{z_N,a_N}\rangle)\colon z_i, a_i \in \{0,1\},\ q_i \in [R],\ q_i \neq q_j, \text{ and } \{q_i, q_j\} \notin E(G^{\mathrm{occ}})\}. \tag{7.124}$$

Note that $\mathcal{I}_\triangle \subset \mathcal{Z}_N(G^\triangle)$ is very similar to $\mathcal{I}(G, G^{\mathrm{occ}}, N) \subset \mathcal{Z}_N(G)$ (from equation (**??**)) but with each single-particle state $|\psi^q_{z,a}\rangle \in \mathcal{Z}_N(G)$ replaced by $|\phi^q_{z,a}\rangle \in \mathcal{Z}_N(G^\triangle)$.

Lemma 28. *The nullspace of $H(G^\triangle, N)$ is $\mathcal{I}_\triangle$ as defined in equation (7.124). Its smallest nonzero eigenvalue is*

$$\gamma(H(G^\triangle, N)) > \frac{1}{(17R)^7}. \tag{7.125}$$

In addition to Fact 2, we use the following simple fact in the proof of the Lemma.

Fact 3. *Let $|p\rangle = c|\alpha_0\rangle + \sqrt{1-c^2}|\alpha_1\rangle$ with $\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$ and $c \in [0,1]$. Then*

$$|p\rangle\langle p| = c^2|\alpha_0\rangle\langle\alpha_0| + M$$

where $\|M\| \leq 1 - \frac{3}{4}c^4$.

To prove this Fact, one can calculate $\|M\| = \frac{1}{2}(1-c^2) + \frac{1}{2}\sqrt{1+2c^2-3c^4}$ and use the inequality $\sqrt{1+x} \leq 1 + \frac{x}{2}$ for $x \geq -1$.

Proof of Lemma 28. Using equation (7.116) and the fact that the smallest eigenvalues of $A(G^\diamondsuit)$ and $A(G^\triangle)$ are the same (equal to e_1, from Section 7.3.5 and Lemma 27), we have

$$H(G^\triangle, N) = H(G^\diamondsuit, N) + \sum_{w=1}^{N} h^{(w)}_{\mathcal{E}^\triangle}\Big|_{\mathcal{Z}_N(G^\triangle)}. \tag{7.126}$$

Recall from Lemma 26 that the nullspace of $H(G^\diamondsuit, N)$ is $\mathcal{I}_\diamondsuit$. We consider

$$\sum_{w=1}^{N} h^{(w)}_{\mathcal{E}^\triangle}\Big|_{\mathcal{I}_\diamondsuit}. \tag{7.127}$$

We show that its nullspace is equal to $\mathcal{I}_\triangle$ (establishing the first part of the Lemma), and we lower bound its smallest nonzero eigenvalue. Specifically, we prove

$$\gamma\left(\sum_{w=1}^{N} h^{(w)}_{\mathcal{E}^\triangle}\Big|_{\mathcal{I}_\diamondsuit}\right) > \frac{1}{(9R)^6}. \tag{7.128}$$

Now we prove equation (7.125) using this bound. We apply the Nullspace Projection Lemma (Lemma **??**) with H_A and H_B given by the first and second terms in equation (7.126); in this case the nullspace of H_A is $S = \mathcal{I}_\diamondsuit$ (from Lemma 26). Now applying Lemma **??** and using the bounds $\gamma(H_A) > \frac{1}{300}$ (from Lemma 26), $\|H_B\| \leq N\|h_{\mathcal{E}^\triangle}\| = 2N \leq 2R$ (from equation (7.21) and the fact that $N \leq R$), and the bound (7.128) on $\gamma(H_B|_S)$, we find

$$\gamma(H(G^\triangle, N)) \geq \frac{\frac{1}{300(9R)^6}}{\frac{1}{300} + \frac{1}{(9R)^6} + 2R} \geq \left(\frac{1}{9^6 + 300 + 600 \cdot 9^6}\right)\frac{1}{R^7} > \frac{1}{(17R)^7}.$$

To complete the proof we must establish that the nullspace of (7.127) is $\mathcal{I}_{\triangle}$ and prove the lower bound (7.128). To analyze (7.127) we use the fact (established in Section 7.3.6) that (7.117) is block diagonal with a block $\mathcal{W}_{(z,a,q)} \subset \mathcal{W}$ for each triple (z, a, q) with $z, a \in \{0, 1\}$ and $q \in [R]$. The operator (7.127) inherits a block structure from this fact. For any basis vector

$$\mathrm{Sym}(|\psi^{q_1}_{z_1,a_1}\rangle|\psi^{q_2}_{z_2,a_2}\rangle \ldots |\psi^{q_N}_{z_N,a_N}\rangle) \in \mathcal{I}_{\diamondsuit}, \tag{7.129}$$

we define a set of occupation numbers

$$\mathcal{N} = \left\{N_{(x,b,r)} \colon x, b \in \{0, 1\},\ r \in [R]\right\}$$

where

$$N_{(x,b,r)} = |\{j \colon |\psi^{q_j}_{z_j,a_j}\rangle \in \mathcal{W}_{(x,b,r)}\}|.$$

Now observe that (7.127) conserves the set of occupation numbers and is therefore block diagonal with a block for each possible set $\mathcal{N}$.

For a given block corresponding to a set of occupation numbers $\mathcal{N}$, we write $\mathcal{I}_{\diamondsuit}(\mathcal{N}) \subset \mathcal{I}_{\diamondsuit}$ for the subspace spanned by basis vectors (7.129) in the block. We classify the blocks into three categories depending on $\mathcal{N}$.

Classification of the blocks of (7.127) according to $\mathcal{N}$

Consider the following two conditions on a set $\mathcal{N} = \{N_{(x,b,r)} \colon x, b \in \{0, 1\},\ r \in [R]\}$ of occupation numbers:

(a) $N_{(x,b,r)} \in \{0, 1\}$ for all $x, b \in \{0, 1\}$ and $r \in [R]$. If this holds, write (y_i, c_i, s_i) for the nonzero occupation numbers (with some arbitrary ordering), i.e., $N_{(y_i,c_i,s_i)} = 1$ for $i \in [N]$.

(b) The sets $\mathcal{W}_{(y_i,c_i,s_i)}$ and $\mathcal{W}_{(y_j,c_j,s_j)}$ do not overlap on a diagram element for all distinct $i, j \in [N]$.

We say a block is of type 1 if $\mathcal{N}$ satisfies (a) and (b). We say it is of type 2 if $\mathcal{N}$ does not satisfy (a). We say it is of type 3 if $\mathcal{N}$ satisfies (a) but does not satisfy (b).

Note that every block is either of type 1, 2, or 3. We consider each type separately. Specifically, we show that each block of type 1 contains one state in the nullspace of (7.127) and, ranging over all blocks of this type, we obtain a basis for $\mathcal{I}_{\triangle}$. We also show that the smallest nonzero eigenvalue within a block of type 1 is at least $\frac{1}{32R^2}$. Finally, we show that blocks of type 2 and 3 do not contain any states in the nullspace of (7.127) and that the smallest eigenvalue within any block of type 2 or 3 is greater than $\frac{1}{(9R)^6}$. Hence, the nullspace of (7.127) is $\mathcal{I}_{\triangle}$ and its smallest nonzero eigenvalue is lower bounded as in equation (7.128).

Type 1

Note (from Definition 12) that (b) implies $q \neq r$ whenever

$$|\psi^{q}_{x,b}\rangle \in \mathcal{W}_{(y_i,c_i,s_i)} \text{ and } |\psi^{r}_{z,a}\rangle \in \mathcal{W}_{(y_j,c_j,s_j)}$$

for distinct $i, j \in [N]$. Hence

$$\begin{aligned}\mathcal{I}_{\diamondsuit}(\mathcal{N}) &= \mathrm{span}\{\mathrm{Sym}(|\psi^{q_1}_{z_1,a_1}\rangle|\psi^{q_2}_{z_2,a_2}\rangle \ldots |\psi^{q_N}_{z_N,a_N}\rangle) \colon q_i \neq q_j \text{ and } |\psi^{q_j}_{z_j,a_j}\rangle \in \mathcal{W}_{(y_j,c_j,s_j)}\} \\ &= \mathrm{span}\{\mathrm{Sym}(|\psi^{q_1}_{z_1,a_1}\rangle|\psi^{q_2}_{z_2,a_2}\rangle \ldots |\psi^{q_N}_{z_N,a_N}\rangle) \colon |\psi^{q_j}_{z_j,a_j}\rangle \in \mathcal{W}_{(y_j,c_j,s_j)}\}.\end{aligned}$$

From this we see that

$$\dim(\mathcal{I}_{\diamondsuit}(\mathcal{N})) = \prod_{j=1}^{N} \left|\mathcal{W}_{(y_j,c_j,s_j)}\right| = \begin{cases}(3R+2)^N & R \text{ odd} \\ (3R-1)^N & R \text{ even.}\end{cases}$$

We now solve for all the eigenstates of (7.127) within the block.

It is convenient to write an orthonormal basis of eigenvectors of the $|\mathcal{W}_{(z,a,q)}| \times |\mathcal{W}_{(z,a,q)}|$ matrix described by Figure **??** as

$$|\phi^q_{z,a}(u)\rangle, \quad u \in [|\mathcal{W}_{(z,a,q)}|] \tag{7.130}$$

and their ordered eigenvalues as

$$\theta_1 \leq \theta_2 \leq \ldots \leq \theta_{|\mathcal{W}_{(z,a,q)}|}.$$

From the proof of Lemma 27, the eigenvector with smallest eigenvalue $\theta_1 = 0$ is $|\phi^q_{z,a}\rangle = |\phi^q_{z,a}(1)\rangle$ and $\theta_2 \geq \frac{1}{32R^2}$. For any $u_1, u_2, \ldots, u_N \in [|\mathcal{W}_{(z,a,q)}|]$, the state

$$\mathrm{Sym}(|\phi^{s_1}_{y_1,c_1}(u_1)\rangle|\phi^{s_2}_{y_2,c_2}(u_2)\rangle \ldots |\phi^{s_N}_{y_N,c_N}(u_N)\rangle)$$

is an eigenvector of (7.127) with eigenvalue $\sum_{j=1}^{N} \theta_j$. Furthermore, states corresponding to different choices of $u_1, \ldots, u_N$ are orthogonal, and ranging over all $\dim(\mathcal{I}_{\diamondsuit}(\mathcal{N}))$ choices we get every eigenvector in the block. The smallest eigenvalue within the block is $N\theta_1 = 0$ and there is a unique vector in the nullspace, given by

$$\mathrm{Sym}(|\phi^{s_1}_{y_1,c_1}\rangle|\phi^{s_2}_{y_2,c_2}\rangle \ldots |\phi^{s_N}_{y_N,c_N}\rangle) \tag{7.131}$$

(recall $|\phi^q_{z,a}\rangle = |\phi^q_{z,a}(1)\rangle$). The smallest nonzero eigenvalue of (7.127) within the block is $(N-1)\theta_1 + \theta_2 = \theta_2 \geq \frac{1}{32R^2}$.

Finally, we show that the collection of states (7.131) obtained from all blocks of type 1 spans the space $\mathcal{I}_{\triangle}$. Each block of type 1 corresponds to a set of occupation numbers

$$N_{(y_1,c_1,s_1)} = N_{(y_2,c_2,s_2)} = \cdots = N_{(y_N,c_N,s_N)} = 1 \quad \text{(with all other occupation numbers zero)}$$

and gives a unique vector (7.131) in the nullspace of $H(G^{\triangle}, N)$. The sets $\mathcal{W}_{(y_i,c_i,s_i)}$ and $\mathcal{W}_{(y_j,c_j,s_j)}$ do not overlap on a diagram element for all distinct $i, j \in [N]$. Using Fact 2 we see this is equivalent to $s_i \neq s_j$ and $\{s_i, s_j\} \notin E(G^{\mathrm{occ}})$ for distinct $i, j \in [N]$. Hence the set of states (7.131) obtained from of all blocks of type 1 is

$$\left\{\mathrm{Sym}(|\phi^{s_1}_{y_1,c_1}\rangle|\phi^{s_2}_{y_2,c_2}\rangle \ldots |\phi^{s_N}_{y_N,c_N}\rangle) \colon y_i, c_i \in \{0,1\},\, s_i \in [R],\, s_i \neq s_j,\, \{s_i, s_j\} \notin E(G^{\mathrm{occ}})\right\}$$

which spans $\mathcal{I}_{\triangle}$.

Type 2

If $\mathcal{N}$ is of type 2 then there exist $x, b \in \{0,1\}$ and $r \in [R]$ such that $N_{(x,b,r)} \geq 2$. We show there are no eigenvectors in the nullspace of (7.127) within a block of this type and we lower bound the smallest eigenvalue within the block. Specifically, we show

$$\min_{|\kappa\rangle \in \mathcal{I}_{\diamond}(\mathcal{N})} \langle\kappa| \sum_{w=1}^{N} h_{\mathcal{E}^{\triangle}}^{(w)} |\kappa\rangle > \frac{1}{(9R)^6}. \tag{7.132}$$

First note that all $|\kappa\rangle \in \mathcal{I}_{\diamond}$ satisfy $(A(G^{\diamond}) - e_1)^{(w)}|\kappa\rangle = 0$ for each $w \in [N]$, which can be seen using the definition of $\mathcal{I}_{\diamond}$ and the fact that $\mathcal{W}$ spans the nullspace of $A(G^{\diamond}) - e_1$. Using this fact and equation (7.116), we get

$$\min_{|\kappa\rangle \in \mathcal{I}_{\diamond}(\mathcal{N})} \langle\kappa| \sum_{w=1}^{N} h_{\mathcal{E}^{\triangle}}^{(w)} |\kappa\rangle = \min_{|\kappa\rangle \in \mathcal{I}_{\diamond}(\mathcal{N})} \langle\kappa| \sum_{w=1}^{N} \left(A(G^{\triangle}) - e_1\right)^{(w)} |\kappa\rangle. \tag{7.133}$$

Now we use the operator inequality

$$\begin{aligned}\sum_{w=1}^{N} \left(A(G^{\triangle}) - e_1\right)^{(w)} &\geq \gamma \left(\sum_{w=1}^{N} \left(A(G^{\triangle}) - e_1\right)^{(w)}\right) \cdot \left(1 - \Pi^{\triangle}\right) \\ &= \gamma(A(G^{\triangle}) - e_1) \cdot \left(1 - \Pi^{\triangle}\right) > \frac{1}{(30R)^2} \left(1 - \Pi^{\triangle}\right),\end{aligned} \tag{7.134}$$

where $\Pi^{\triangle}$ is the projector onto the nullspace of $\sum_{w=1}^{N} \left(A(G^{\triangle}) - e_1\right)^{(w)}$, and where in the last step we used Lemma 27. Plugging equation (7.134) into equation (7.133) gives

$$\min_{|\kappa\rangle \in \mathcal{I}_{\diamond}(\mathcal{N})} \langle\kappa| \sum_{w=1}^{N} h_{\mathcal{E}^{\triangle}}^{(w)} |\kappa\rangle > \frac{1}{(30R)^2} \Big(1 - \max_{|\kappa\rangle \in \mathcal{I}_{\diamond}(\mathcal{N})} \langle\kappa|\Pi^{\triangle}|\kappa\rangle\Big). \tag{7.135}$$

In the following we show that $\langle\kappa|\Pi^{\triangle}|\kappa\rangle = \langle\kappa|\Pi^{\triangle}_{\mathcal{N}}|\kappa\rangle$ for all $|\kappa\rangle \in \mathcal{I}_{\diamond}(\mathcal{N})$, where $\Pi^{\triangle}_{\mathcal{N}}$ is a Hermitian operator with

$$1 - \left\|\Pi^{\triangle}_{\mathcal{N}}\right\| \geq \frac{3}{4}\left(\frac{1}{4R}\right)^4 = \frac{3}{1024R^4}. \tag{7.136}$$

Plugging this into (7.135) gives

$$\min_{|\kappa\rangle \in \mathcal{I}_{\diamond}(\mathcal{N})} \langle\kappa| \sum_{w=1}^{N} h_{\mathcal{E}^{\triangle}}^{(w)} |\kappa\rangle > \frac{3}{(30R)^2 \cdot 1024R^4} > \frac{1}{(9R)^6}.$$

To complete the proof, we exhibit the operator $\Pi^{\triangle}_{\mathcal{N}}$ and show that its norm is bounded as (7.136). Using Lemma 27 we can write $\Pi^{\triangle}$ explicitly as

$$\Pi^{\triangle} = \sum_{(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}} \mathcal{P}_{(\vec{z},\vec{a},\vec{q})} \tag{7.137}$$

where

$$\mathcal{P}_{(\vec{z},\vec{a},\vec{q})} = |\phi^{q_1}_{z_1,a_1}\rangle\langle\phi^{q_1}_{z_1,a_1}| \otimes |\phi^{q_2}_{z_2,a_2}\rangle\langle\phi^{q_2}_{z_2,a_2}| \otimes \cdots \otimes |\phi^{q_N}_{z_N,a_N}\rangle\langle\phi^{q_N}_{z_N,a_N}|$$
$$\mathcal{Q} = \{(z_1, \ldots z_N, a_1, \ldots, a_N, q_1, \ldots, q_N) : \; z_i, a_i \in \{0,1\} \text{ and } q_i \in [R]\}.$$

For each $(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}$ we also define a space

$$S_{(\vec{z},\vec{a},\vec{q})} = \operatorname{span}(\mathcal{W}_{(z_1,a_1,q_1)}) \otimes \operatorname{span}(\mathcal{W}_{(z_2,a_2,q_2)}) \otimes \cdots \otimes \operatorname{span}(\mathcal{W}_{(z_N,a_N,q_N)}).$$

Note that $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}$ has all of its support in $S_{(\vec{z},\vec{a},\vec{q})}$, and that

$$S_{(\vec{z},\vec{a},\vec{q})} \perp S_{(\vec{z}',\vec{a}',\vec{q}')} \text{ for distinct } (\vec{z},\vec{a},\vec{q}), (\vec{z}',\vec{a}',\vec{q}') \in \mathcal{Q}. \tag{7.138}$$

Therefore $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}\mathcal{P}_{(\vec{z}',\vec{a}',\vec{q}')} = 0$ for distinct $(\vec{z},\vec{a},\vec{q}), (\vec{z}',\vec{a}',\vec{q}') \in \mathcal{Q}$. (Below we use similar reasoning to obtain a less obvious result.) Note that $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}$ is orthogonal to $\mathcal{I}_{\diamondsuit}(\mathcal{N})$ unless

$$|\{j : (z_j, a_j, q_j) = (w, u, v)\}| = N_{(w,u,v)} \text{ for all } w, u \in \{0,1\},\ v \in [R]. \tag{7.139}$$

We restrict our attention to the projectors that are not orthogonal to $\mathcal{I}_{\diamondsuit}(\mathcal{N})$. Letting $\mathcal{Q}(\mathcal{N}) \subset \mathcal{Q}$ be the set of $(\vec{z},\vec{a},\vec{q})$ satisfying equation (7.139), we have

$$\langle\kappa| \sum_{(\vec{z},\vec{a},\vec{q})\in\mathcal{Q}} \mathcal{P}_{(\vec{z},\vec{a},\vec{q})}|\kappa\rangle = \langle\kappa| \sum_{(\vec{z},\vec{a},\vec{q})\in\mathcal{Q}(\mathcal{N})} \mathcal{P}_{(\vec{z},\vec{a},\vec{q})}|\kappa\rangle \quad \text{for all } |\kappa\rangle \in \mathcal{I}_{\diamondsuit}(\mathcal{N}). \tag{7.140}$$

Since $N_{(x,b,r)} \geq 2$, note that in each term $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}$ with $(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}(\mathcal{N})$, the operator

$$|\phi^r_{x,b}\rangle\langle\phi^r_{x,b}| \otimes |\phi^r_{x,b}\rangle\langle\phi^r_{x,b}|$$

appears between two of the N registers (tensored with rank-1 projectors on the other $N-2$ registers). Using equation (7.122) we may expand $|\phi^r_{x,b}\rangle$ as a sum of states from $\mathcal{W}_{(x,b,r)}$. This gives

$$|\phi^r_{x,b}\rangle|\phi^r_{x,b}\rangle = c_0|\psi^{r_{\text{in}}}_{x,b}\rangle|\psi^{r_{\text{in}}}_{x,b}\rangle + \left(1 - c_0^2\right)^{\frac{1}{2}} |\Phi^r_{x,b}\rangle$$

where c_0 is either $\frac{1}{3R+2}$ (if R is odd) or $\frac{1}{3R-1}$ (if R is even), and where $|\psi^{r_{\text{in}}}_{x,b}\rangle|\psi^{r_{\text{in}}}_{x,b}\rangle$ is orthogonal to $|\Phi^r_{x,b}\rangle$. Note that each of the states $|\phi^r_{x,b}\rangle|\phi^r_{x,b}\rangle$, $|\psi^{r_{\text{in}}}_{x,b}\rangle|\psi^{r_{\text{in}}}_{x,b}\rangle$, and $|\Phi^r_{x,b}\rangle$ lie in the space

$$\operatorname{span}(\mathcal{W}_{(x,b,r)}) \otimes \operatorname{span}(\mathcal{W}_{(x,b,r)}). \tag{7.141}$$

Now applying Fact 3 gives

$$|\phi^r_{x,b}\rangle\langle\phi^r_{x,b}| \otimes |\phi^r_{x,b}\rangle\langle\phi^r_{x,b}| = c_0^2|\psi^{r_{\text{in}}}_{x,b}\rangle\langle\psi^{r_{\text{in}}}_{x,b}| \otimes |\psi^{r_{\text{in}}}_{x,b}\rangle\langle\psi^{r_{\text{in}}}_{x,b}| + M^r_{x,b} \tag{7.142}$$

where $M^r_{x,b}$ is a Hermitian operator with all of its support on the space (7.141) and

$$\left\|M^r_{x,b}\right\| \leq 1 - \frac{3}{4}c_0^4 \leq 1 - \frac{3}{4}\left(\frac{1}{3R+2}\right)^4 \leq 1 - \frac{3}{4}\frac{1}{(4R)^4} \tag{7.143}$$

since $R \geq 2$. For each $(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}(\mathcal{N})$ we define $\mathcal{P}^M_{(\vec{z},\vec{a},\vec{q})}$ to be the operator obtained from $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}$ by replacing

$$|\phi^r_{x,b}\rangle\langle\phi^r_{x,b}| \otimes |\phi^r_{x,b}\rangle\langle\phi^r_{x,b}| \mapsto M^r_{x,b}$$

on two of the registers (if $N_{(x,b,r)} > 2$ there is more than one way to do this; we fix one choice for each $(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}(\mathcal{N})$). Note that $\mathcal{P}^M_{(\vec{z},\vec{a},\vec{q})}$ has all of its support in the space $S_{(\vec{z},\vec{a},\vec{q})}$. Using (7.138) gives

$$\mathcal{P}^M_{(\vec{z},\vec{a},\vec{q})}\mathcal{P}^M_{(\vec{z}',\vec{a}',\vec{q}')} = 0 \text{ for distinct } (\vec{z},\vec{a},\vec{q}),(\vec{z}',\vec{a}',\vec{q}') \in \mathcal{Q}(\mathcal{N}).$$

Using equation (7.142) and the fact that

$$\langle\kappa|\Big(|\psi^{r_{\mathrm{in}}}_{x,b}\rangle\langle\psi^{r_{\mathrm{in}}}_{x,b}|^{(w_1)}\Big)\Big(|\psi^{r_{\mathrm{in}}}_{x,b}\rangle\langle\psi^{r_{\mathrm{in}}}_{x,b}|^{(w_2)}\Big)|\kappa\rangle = 0 \quad \text{for all } |\kappa\rangle \in \mathcal{I}_\Diamond(\mathcal{N}) \text{ and distinct } w_1, w_2 \in [N]$$

(which can be seen from the definition of $\mathcal{I}_\Diamond$), we have

$$\langle\kappa|\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}|\kappa\rangle = \langle\kappa|\mathcal{P}^M_{(\vec{z},\vec{a},\vec{q})}|\kappa\rangle \quad \text{for all } |\kappa\rangle \in \mathcal{I}_\Diamond(\mathcal{N}).$$

Hence, letting

$$\Pi^{\triangle}_{\mathcal{N}} = \sum_{(\vec{z},\vec{a},\vec{q})\in\mathcal{Q}(\mathcal{N})} \mathcal{P}^M_{(\vec{z},\vec{a},\vec{q})}, \tag{7.144}$$

we have $\langle\kappa|\Pi^{\triangle}|\kappa\rangle = \langle\kappa|\Pi^{\triangle}_{\mathcal{N}}|\kappa\rangle$ for all $|\kappa\rangle \in \mathcal{I}_\Diamond(\mathcal{N})$. To obtain the desired bound (7.136) on the norm of $\Pi^{\triangle}_{\mathcal{N}}$, we use the fact that the norm of a sum of pairwise orthogonal Hermitian operators is upper bounded by the maximum norm of an operator in the sum, so

$$\left\|\Pi^{\triangle}_{\mathcal{N}}\right\| = \left\|\sum_{(\vec{z},\vec{a},\vec{q})\in\mathcal{Q}(\mathcal{N})} \mathcal{P}^M_{(\vec{z},\vec{a},\vec{q})}\right\| = \max_{(\vec{z},\vec{a},\vec{q})\in\mathcal{Q}(\mathcal{N})} \left\|\mathcal{P}^M_{(\vec{z},\vec{a},\vec{q})}\right\| = \left\|M^r_{x,b}\right\| \leq 1 - \frac{3}{4}\frac{1}{(4R)^4}. \tag{7.145}$$

Type 3

If $\mathcal{N}$ is of type 3 then $N_{(x,b,r)} \in \{0,1\}$ for all $x, b \in \{0,1\}$ and $r \in [R]$, and

$$N_{(y,c,s)} = N_{(t,d,u)} = 1$$

for some $(y,c,s) \neq (t,d,u)$ with either $u = s$ or $\{u,s\} \in E(G^{\mathrm{occ}})$ (using property (b) and Fact 2). We show there are no eigenvectors in the nullspace of (7.127) within a block of this type and we lower bound the smallest eigenvalue within the block. We establish the same bound (7.132) as for blocks of Type 2.

The proof is very similar to that given above for blocks of Type 2. In fact, the first part of proof is identical, from equation (7.133) up to and including equation (7.140). That is to say, as in the previous case we have

$$\langle\kappa|\sum_{(\vec{z},\vec{a},\vec{q})\in\mathcal{Q}} \mathcal{P}_{(\vec{z},\vec{a},\vec{q})}|\kappa\rangle = \langle\kappa|\sum_{(\vec{z},\vec{a},\vec{q})\in\mathcal{Q}(\mathcal{N})} \mathcal{P}_{(\vec{z},\vec{a},\vec{q})}|\kappa\rangle \quad \text{for all } |\kappa\rangle \in \mathcal{I}_\Diamond(\mathcal{N}). \tag{7.146}$$

In this case, since $N_{(y,c,s)} = N_{(t,d,u)} = 1$, in each term $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}$ with $(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}(\mathcal{N})$, the operator

$$|\phi^s_{y,c}\rangle\langle\phi^s_{y,c}| \otimes |\phi^u_{t,d}\rangle\langle\phi^u_{t,d}|$$

appears between two of the N registers (tensored with rank 1 projectors on the other $N-2$ registers). Using equation (7.122) we may expand $|\phi^s_{y,c}\rangle$ and $|\phi^u_{t,d}\rangle$ as superpositions (with amplitudes $\pm\frac{1}{\sqrt{3R+2}}$ if R is odd or $\pm\frac{1}{\sqrt{3R-1}}$ if R is even) of the basis states from $\mathcal{W}_{(y,c,s)}$ and $\mathcal{W}_{(t,d,u)}$ respectively. Since $\mathcal{W}_{(y,c,s)}$ and $\mathcal{W}_{(t,d,u)}$ overlap on some diagram element, there exists $l \in L^{\square}$ such that $|\psi^l_{x_1,b_1}\rangle \in \mathcal{W}_{(y,c,s)}$ and $|\psi^l_{x_2,b_2}\rangle \in \mathcal{W}_{(t,d,u)}$ for some $x_1, x_2, b_1, b_2 \in \{0,1\}$. Hence

$$|\phi^s_{y,c}\rangle|\phi^u_{t,d}\rangle = c_0\left(\pm|\psi^l_{x_1,b_1}\rangle|\psi^l_{x_2,b_2}\rangle\right) + \left(1-c_0^2\right)^{\frac{1}{2}}|\Phi^{s,u}_{y,c,t,d}\rangle$$

where c_0 is either $\frac{1}{3R+2}$ (if R is odd) or $\frac{1}{3R-1}$ (if R is even). Now applying Fact 3 we get

$$|\phi^s_{y,c}\rangle\langle\phi^s_{y,c}| \otimes |\phi^u_{t,d}\rangle\langle\phi^u_{t,d}| = c_0^2|\psi^l_{x_1,b_1}\rangle\langle\psi^l_{x_1,b_1}| \otimes |\psi^l_{x_2,b_2}\rangle\langle\psi^l_{x_2,b_2}| + M^{s,u}_{y,c,t,d} \tag{7.147}$$

where $\|M^{s,u}_{y,c,t,d}\| \le 1-\frac{3}{4}\left(\frac{1}{4R}\right)^4$. For each $(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}(\mathcal{N})$ we define $\mathcal{P}^M_{(\vec{z},\vec{a},\vec{q})}$ to be the operator obtained from $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}$ by replacing

$$|\phi^s_{y,c}\rangle\langle\phi^s_{y,c}| \otimes |\phi^u_{t,d}\rangle\langle\phi^u_{t,d}| \mapsto M^{s,u}_{y,c,t,d}$$

on two of the registers and we let $\Pi^{\triangle}_{\mathcal{N}}$ be given by (7.144). Then, as in the previous case, $\langle\kappa|\Pi^{\triangle}|\kappa\rangle = \langle\kappa|\Pi^{\triangle}_{\mathcal{N}}|\kappa\rangle$ for all $|\kappa\rangle \in \mathcal{I}_{\diamondsuit}(\mathcal{N})$ and using the same reasoning as before, we get the bound (7.136) on $\|\Pi^{\triangle}_{\mathcal{N}}\|$. Using these two facts we get the same bound on the smallest eigenvalue within a block of type 3 as the bound we obtained for blocks of type 2:

$$\min_{|\kappa\rangle\in\mathcal{I}_{\diamondsuit}(\mathcal{N})}\langle\kappa|\sum_{w=1}^{N}h^{(w)}_{\mathcal{E}^{\triangle}}|\kappa\rangle > \frac{1}{(30R)^2}\left(1-\left\|\Pi^{\triangle}_{\mathcal{N}}\right\|\right) > \frac{1}{(9R)^6}.$$

□

7.3.8 The gate graph $G^{\square}$

We now consider the gate graph $G^{\square}$ and prove Lemma ??. We first show that $G^{\square}$ is an e_1-gate graph. From equations (7.108), (7.109), and (7.110) we have

$$A(G^{\square}) = A(G^{\triangle}) + h_{\mathcal{E}^0} + h_{\mathcal{S}^0}. \tag{7.148}$$

Lemma 27 characterizes the e_1-energy ground space of $G^{\triangle}$ and gives an orthonormal basis $\{|\phi^q_{z,a}\rangle\colon z,a \in \{0,1\},\ q \in [R]\}$ for it. To solve for the e_1-energy ground space of $A(G^{\square})$, we solve for superpositions of the states $\{|\phi^q_{z,a}\rangle\}$ in the nullspace of $h_{\mathcal{E}^0} + h_{\mathcal{S}^0}$.

Recall the definition of the sets $\mathcal{E}^0$ and $\mathcal{S}^0$. From Section 7.3.4.1, each node (q,z,t) in the gate diagram for G is associated with a node $\mathrm{new}(q,z,t)$ in the gate diagram for $G^{\square}$ as described by (7.103). This mapping is depicted in Figure ?? by the black and grey arrows. Applying this mapping to each pair of nodes in the edge set $\mathcal{E}^G$ and each node in the self-loop set $\mathcal{S}^G$ of the gate diagram for G, we get the sets $\mathcal{E}^0$ and $\mathcal{S}^0$. Hence, using equations (7.18) and (7.19),

$$h_{\mathcal{S}^0} = \sum_{(q,z,t)\in\mathcal{S}^G}|\mathrm{new}(q,z,t)\rangle\langle\mathrm{new}(q,z,t)| \otimes \mathbb{I} \tag{7.149}$$

$$h_{\mathcal{E}^0} = \sum_{\{(q,z,t),(q',z',t')\}\in\mathcal{E}^G}\left(|\mathrm{new}(q,z,t)\rangle + |\mathrm{new}(q',z',t')\rangle\right)\left(\langle\mathrm{new}(q,z,t)| + \langle\mathrm{new}(q',z',t')|\right) \otimes \mathbb{I}. \tag{7.150}$$

Using equation (7.122), we see that for all nodes (q,z,t) in the gate diagram for G and for all $j \in \{0,\ldots,7\}$, $x,b \in \{0,1\}$, and $r \in [R]$,

$$\begin{aligned} \langle \text{new}(q,z,t), j|\phi^r_{x,b}\rangle &= \sqrt{c_0}\begin{cases} \langle q_{\text{in}}, z, t, j|\psi^{r_{\text{in}}}_{x,b}\rangle & \text{if } (q,z,t) \text{ is an input node} \\ \langle q_{\text{out}}, z, t, j|\psi^{r_{\text{out}}}_{x,b}\rangle & \text{if } (q,z,t) \text{ is an output node} \end{cases} \\ &= \sqrt{c_0}\delta_{r,q}\langle z,t,j|\psi_{x,b}\rangle \end{aligned} \tag{7.151}$$

where c_0 is $\frac{1}{3R+2}$ if R is odd or $\frac{1}{3R-1}$ if R is even, and where $|\psi_{x,b}\rangle$ is defined by equations (7.15) and (7.16). The matrix element on the left-hand side of this equation is evaluated in the Hilbert space $\mathcal{Z}_1(G^\square)$ where each basis vector corresponds to a vertex of the graph $G^\square$; these vertices are labeled (l,z,t,j) with $l \in L^\square$, $z \in \{0,1\}$, $t \in [8]$, and $j \in \{0,\ldots,7\}$. However, from (7.151) we see that

$$\underbrace{\langle \text{new}(q,z,t), j|\phi^r_{x,b}\rangle}_{\text{in } \mathcal{Z}_1(G^\square)} = \sqrt{c_0}\,\underbrace{\langle q,z,t,j|\psi^r_{x,b}\rangle}_{\text{in } \mathcal{Z}_1(G)} \tag{7.152}$$

where the right-hand side is evaluated in the Hilbert space $\mathcal{Z}_1(G)$.

Putting together equations (7.149), (7.150), and (7.152) gives

$$\langle \phi^q_{z,a}|h_{\mathcal{E}^0} + h_{\mathcal{S}^0}|\phi^r_{x,b}\rangle = \langle \psi^q_{z,a}|h_{\mathcal{E}^G} + h_{\mathcal{S}^G}|\psi^r_{x,b}\rangle \cdot \begin{cases} \frac{1}{3R+2} & R \text{ odd} \\ \frac{1}{3R-1} & R \text{ even} \end{cases} \tag{7.153}$$

for all $z,a,x,b \in \{0,1\}$ and $q,r \in [R]$. On the left-hand side of this equation, the Hilbert space is $\mathcal{Z}_1(G^\square)$; on the right-hand side it is $\mathcal{Z}_1(G)$.

We use equation (7.153) to relate the e_1-energy ground states of $A(G)$ to those of $A(G^\square)$. Since G is an e_1-gate graph, there is a state

$$|\Gamma\rangle = \sum_{z,a,q} \alpha_{z,a,q}|\psi^q_{z,a}\rangle \in \mathcal{Z}_1(G)$$

that satisfies $A(G)|\Gamma\rangle = e_1|\Gamma\rangle$ and hence $h_{\mathcal{E}^G}|\Gamma\rangle = h_{\mathcal{S}^G}|\Gamma\rangle = 0$. Letting

$$|\Gamma'\rangle = \sum_{z,a,q} \alpha_{z,a,q}|\phi^q_{z,a}\rangle \in \mathcal{Z}_1(G^\square)$$

and using equation (7.153), we see that $\langle \Gamma'|h_{\mathcal{E}^0} + h_{\mathcal{S}^0}|\Gamma'\rangle = 0$ and therefore $\langle \Gamma'|A(G^\square)|\Gamma'\rangle = e_1$. Hence $G^\square$ is an e_1-gate graph. Moreover, the linear mapping from $\mathcal{Z}_1(G)$ to $\mathcal{Z}_1(G^\square)$ defined by

$$|\psi^q_{z,a}\rangle \mapsto |\phi^q_{z,a}\rangle \tag{7.154}$$

maps each e_1-energy eigenstate of $A(G)$ to an e_1-energy eigenstate of $A(G^\square)$.

Now consider the N-particle Hamiltonian $H(G^\square, N)$. Using equation (7.148) and the fact that both $A(G^\square)$ and $A(G^\triangle)$ have smallest eigenvalue e_1, we have

$$H(G^\square, N) = H(G^\triangle, N) + \sum_{w=1}^{N} \left(h_{\mathcal{E}^0} + h_{\mathcal{S}^0}\right)^{(w)}\Big|_{\mathcal{Z}_N(G^\square)}.$$

Recall from Lemma 27 that the nullspace of the first term is $\mathcal{I}_\triangle$. The N-fold tensor product of the mapping (7.154) acts on basis vectors of $\mathcal{I}(G, G^{\mathrm{occ}}, N)$ as

$$\mathrm{Sym}(|\psi^{q_1}_{z_1,a_1}\rangle|\psi^{q_2}_{z_2,a_2}\rangle \ldots |\psi^{q_N}_{z_N,a_N}\rangle) \mapsto \mathrm{Sym}(|\phi^{q_1}_{z_1,a_1}\rangle|\phi^{q_2}_{z_2,a_2}\rangle \ldots |\phi^{q_N}_{z_N,a_N}\rangle), \tag{7.155}$$

where $z_i, a_i \in \{0,1\}$, $q_i \neq q_j$, and $\{q_i, q_j\} \notin E(G^{\mathrm{occ}})$. Clearly this defines an invertible linear map between the two spaces $\mathcal{I}(G, G^{\mathrm{occ}}, N)$ and $\mathcal{I}_\triangle$. Let $|\Theta\rangle \in \mathcal{I}(G, G^{\mathrm{occ}}, N)$ and write $|\Theta'\rangle \in \mathcal{I}_\triangle$ for its image under the map (7.155). Then

$$\langle\Theta'|H(G^\square, N)|\Theta'\rangle = \langle\Theta'|\sum_{w=1}^{N}(h_{\mathcal{E}^0} + h_{\mathcal{S}^0})^{(w)}|\Theta'\rangle = \langle\Theta|\sum_{w=1}^{N}(h_{\mathcal{E}^G} + h_{\mathcal{S}^G})^{(w)}|\Theta\rangle \cdot \begin{cases} \frac{1}{3R+2} & R \text{ odd} \\ \frac{1}{3R-1} & R \text{ even} \end{cases} \tag{7.156}$$

where in the first equality we used the fact that $|\Theta'\rangle$ is in the nullspace $\mathcal{I}_\triangle$ of $H(G^\triangle, N)$ and in the second equality we used equation (7.153) and the fact that $\langle\phi^q_{z,a}|\phi^r_{x,b}\rangle = \langle\psi^q_{z,a}|\psi^r_{x,b}\rangle$. We now complete the proof of Lemma **??** using equation (7.156).

Case 1: $\lambda_N(G, G^{\mathbf{occ}}) \leq a$

In this case there exists a state $|\Theta\rangle \in \mathcal{I}(G, G^{\mathrm{occ}}, N)$ satisfying

$$\langle\Theta|\sum_{w=1}^{N}(h_{\mathcal{E}^G} + h_{\mathcal{S}^G})^{(w)}|\Theta\rangle \leq a.$$

From equation (7.156) we see that the state $|\Theta'\rangle \in \mathcal{I}_\triangle$ satisfies $\langle\Theta'|H(G^\square, N)|\Theta'\rangle \leq \frac{a}{3R-1} \leq \frac{a}{R}$.

Case 2: $\lambda_N(G, G^{\mathbf{occ}}) \geq b$

In this case

$$\lambda_N(G, G^{\mathrm{occ}}) = \min_{|\Theta\rangle \in \mathcal{I}(G,G^{\mathrm{occ}},N)} \langle\Theta|H(G, G^{\mathrm{occ}}, N)|\Theta\rangle = \min_{|\Theta\rangle \in \mathcal{I}(G,G^{\mathrm{occ}},N)} \langle\Theta|\sum_{w=1}^{N}(h_{\mathcal{E}^G} + h_{\mathcal{S}^G})^{(w)}|\Theta\rangle \geq b.$$

Now applying equation (7.156) gives

$$\min_{|\Theta'\rangle \in \mathcal{I}_\triangle} \langle\Theta'|H(G^\square, N)|\Theta'\rangle = \min_{|\Theta'\rangle \in \mathcal{I}_\triangle} \langle\Theta'|\sum_{w=1}^{N}(h_{\mathcal{E}^0} + h_{\mathcal{S}^0})^{(w)}|\Theta'\rangle \geq \frac{1}{3R+2} b. \tag{7.157}$$

This establishes that the nullspace of $H(G^\square, N)$ is empty, i.e., $\lambda^1_N(G^\square) > 0$, so $\lambda^1_N(G^\square) = \gamma(H(G^\square, N))$. We lower bound $\lambda^1_N(G^\square)$ using the Nullspace Projection Lemma (Lemma **??**) with

$$H_A = H(G^\triangle, N) \qquad H_B = \sum_{w=1}^{N}(h_{\mathcal{E}^0} + h_{\mathcal{S}^0})^{(w)}\Big|_{\mathcal{Z}_N(G^\square)}$$

and where the nullspace of H_A is $S = \mathcal{I}_\triangle$. We apply Lemma **??** and use the bounds $\gamma(H_A) > \frac{1}{(17R)^7}$ (from Lemma 28), $\gamma(H_B|_S) \geq \frac{b}{3R+2}$ (from equation (7.157)), and $\|H_B\| \leq$

$N \left\| h_{\mathcal{E}^0} + h_{\mathcal{S}^0} \right\| \leq 3N \leq 3R$ (using equations (7.21) and (7.20) and the fact that $N \leq R$) to find

$$\begin{aligned}
\lambda_N^1(G^\square) &= \gamma(H(G^\square, N)) \\
&\geq \frac{b}{(3R+2)(17R)^7(\frac{1}{(17R)^7} + \frac{b}{3R+2} + 3R)} \\
&\geq \frac{b}{R^9} \cdot \frac{1}{3 + 2 + b \cdot (17)^7 + 3 \cdot (3+2)\,(17)^7} \\
&> \frac{b}{(13R)^9}
\end{aligned}$$

where in the denominator we used the fact that $b \leq 1$.

7.3.9 Completeness and Soundness

Well fuck.

7.4 Discussion and open problems

While these results generalized the problem of the Bose-Hubbard model to arbitrary interactions between bosons, it leaves open the related question of fermions. I would expect that our proof would naturally extend to fermions as well, but the extensions where too extensive to finish in time for this thesis.

Making the eventual graph regular.

Remove the restriction to fixed particle number. Currently, this corresponds to

Chapter 8

Ground energy of spin systems

We reduce Frustration-Free Bose-Hubbard Hamiltonian to an eigenvalue problem for a class of 2-local Hamiltonians defined by graphs. The reduction is based on a well-known mapping between hard-core bosons and spin systems, which we now review.

We define the subspace $\mathcal{W}_N(G) \subset \mathcal{Z}_N(G)$ of N hard-core bosons on a graph G to consist of the states where each vertex of G is occupied by either 0 or 1 particle, i.e.,

$$\mathcal{W}_N(G) = \mathrm{span}\{\mathrm{Sym}(|i_1, i_2, \ldots, i_N\rangle) \colon i_1, \ldots, i_N \in V,\ i_j \neq i_k \text{ for distinct } j, k \in [N]\}.$$

A basis for $\mathcal{W}_N(G)$ is the subset of occupation-number states (**??**) labeled by bit strings $l_1 \ldots l_{|V|} \in \{0,1\}^{|V|}$ with Hamming weight $\sum_{j \in V} l_j = N$. The space $\mathcal{W}_N(G)$ can thus be identified with the weight-N subspace

$$\mathrm{Wt}_N(G) = \mathrm{span}\{|z_1, \ldots, z_{|V|}\rangle :\ z_i \in \{0,1\},\ \sum_{i=1}^{|V|} z_i = N\}$$

of a $|V|$-qubit Hilbert space. We consider the restriction of H_G^N to the space $\mathcal{W}_N(G)$, which can equivalently be written as a $|V|$-qubit Hamiltonian O_G restricted to the space $\mathrm{Wt}_N(G)$. In particular,

$$H_G^N\big|_{\mathcal{W}_N(G)} = O_G\big|_{\mathrm{Wt}_N(G)} \tag{8.1}$$

where

$$\begin{aligned} O_G &= \sum_{\substack{A(G)_{ij}=1 \\ i \neq j}} \big(|01\rangle\langle 10| + |10\rangle\langle 01|\big)_{ij} + \sum_{A(G)_{ii}=1} |1\rangle\langle 1|_i \\ &= \sum_{\substack{A(G)_{ij}=1 \\ i \neq j}} \frac{\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j}{2} + \sum_{A(G)_{ii}=1} \frac{1 - \sigma_z^i}{2}. \end{aligned}$$

Note that the Hamiltonian O_G conserves the total magnetization $M_z = \sum_{1=1}^{|V|} \frac{1-\sigma_z^i}{2}$ along the z axis.

We define $\theta_N(G)$ to be the smallest eigenvalue of (8.1), i.e., the ground energy of O_G in the sector with magnetization N. We show that approximating this quantity is QMA-complete.

Problem 4 (**XY Hamiltonian**)**.** We are given a K-vertex graph G, an integer $N \leq K$, a real number c, and a precision parameter $\epsilon = \frac{1}{T}$. The positive integer T is provided in unary; the graph is specified by its adjacency matrix, which can be any $K \times K$ symmetric 0-1 matrix. We are promised that either $\theta_N(G) \leq c$ (yes instance) or else $\theta_N(G) \geq c + \epsilon$ (no instance) and we are asked to decide which is the case.

8.1 Relation between spins and particles

8.1.1 The transform

8.2 Hardness reduction from frustration-free BH model

Theorem 3. *XY Hamiltonian is QMA-complete.*

Proof. An instance of XY Hamiltonian can be verified by the standard QMA verification protocol for the Local Hamiltonian problem [**?**] with one slight modification: before running the protocol Arthur measures the magnetization of the witness and rejects unless it is equal to N. Thus the problem is contained in QMA.

To prove QMA-hardness, we show that the solution (yes or no) of an instance of Frustration-Free Bose-Hubbard Hamiltonian with input G, N, ϵ is equal to the solution of the instance of XY Hamiltonian with the same graph G and integer N, with precision parameter $\frac{\epsilon}{4}$ and $c = N\mu(G) + \frac{\epsilon}{4}$.

We separately consider yes instances and no instances of Frustration-Free Bose-Hubbard Hamiltonian and show that the corresponding instance of XY Hamiltonian has the same solution in both cases.

Case 1: no instances

First consider a no instance of Frustration-Free Bose-Hubbard Hamiltonian, for which $\lambda_N^1(G) \geq \epsilon + \epsilon^3$. We have

$$\lambda_N^1(G) = \min_{\substack{|\phi\rangle \in \mathcal{Z}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi|H_G^N - N\mu(G)|\phi\rangle \tag{8.2}$$

$$\leq \min_{\substack{|\phi\rangle \in \mathcal{W}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi|H_G^N - N\mu(G)|\phi\rangle \tag{8.3}$$

$$= \min_{\substack{|\phi\rangle \in \mathrm{Wt}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi|O_G - N\mu(G)|\phi\rangle \tag{8.4}$$

$$= \theta_N(G) - N\mu(G) \tag{8.5}$$

where in the inequality we used the fact that $\mathcal{W}_N(G) \subset \mathcal{Z}_N(G)$. Hence

$$\theta_N(G) \geq N\mu(G) + \lambda_N^1(G) \geq N\mu(G) + \epsilon + \epsilon^3 \geq N\mu(G) + \frac{\epsilon}{2},$$

so the corresponding instance of XY Hamiltonian is a no instance.

Case 2: yes instances

Now consider a yes instance of Frustration-Free Bose-Hubbard Hamiltonian, so $0 \leq \lambda_N^1(G) \leq \epsilon^3$.

We consider the case $\lambda_N^1(G) = 0$ separately from the case where it is strictly positive. If $\lambda_N^1(G) = 0$ then any state $|\psi\rangle$ in the ground space of H_G^N satisfies

$$\langle\phi| \sum_{w=1}^{N} (A(G) - \mu(G))^{(w)} + \sum_{k \in V} \widehat{n}_k(\widehat{n}_k - 1) |\phi\rangle = 0.$$

Since both terms are positive semidefinite, the state $|\phi\rangle$ has zero energy for each of them. In particular, it has zero energy for the second term, or equivalently, $|\phi\rangle \in \mathcal{W}_N(G)$. Therefore

$$\lambda_N^1(G) = \min_{\substack{|\phi\rangle \in \mathcal{W}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi| H_G^N - N\mu(G) |\phi\rangle = \min_{\substack{|\phi\rangle \in \mathrm{Wt}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi| O_G - N\mu(G) |\phi\rangle = \theta_N(G) - N\mu(G),$$

so $\theta_N(G) = N\mu(G)$, and the corresponding instance of XY Hamiltonian is a yes instance.

Finally, suppose $0 < \lambda_N^1(G) \leq \epsilon^3$. Then $\lambda_N^1(G)$ is also the smallest *nonzero* eigenvalue of $H(G, N)$, which we denote by $\gamma(H(G, N))$. (Here and throughout this paper we write $\gamma(M)$ for the smallest nonzero eigenvalue of a positive semidefinite matrix M.) Note that $\lambda_N^1(G) > 0$ also implies (by the inequalities (8.2)–(8.5)) that $\theta_N(G) - N\mu(G) > 0$, so

$$\theta_N(G) - N\mu(G) = \gamma\left((O_G - N\mu(G))\big|_{\mathrm{Wt}_N(G)} \right).$$

To upper bound $\theta_N(G)$ we use the Nullspace Projection Lemma (Lemma **??**). We apply this Lemma using the decomposition $H(G, N) = H_A + H_B$ where

$$H_A = \sum_{k \in V} \widehat{n}_k(\widehat{n}_k - 1)\big|_{\mathcal{Z}_N(G)} \qquad H_B = \sum_{w=1}^{N} (A(G) - \mu(G))^{(w)}\big|_{\mathcal{Z}_N(G)}.$$

Note that H_A and H_B are both positive semidefinite, and that the nullspace S of H_A is equal the space $\mathcal{W}_N(G)$ of hard-core bosons. To apply the Lemma we compute bounds on $\gamma(H_A)$, $\|H_B\|$, and $\gamma(H_B|_S)$. We use the bounds $\gamma(H_A) = 2$ (since the operators $\{\widehat{n}_k \colon k \in V\}$ commute and have nonnegative integer eigenvalues),

$$\|H_B\| \leq N\|A(G) - \mu(G)\| \leq N(\|A(G)\| + \mu(G)) \leq 2N\|A(G)\| \leq 2KN \leq 2K^2$$

(where we used the fact that $\|A(G)\|$ is at most the maximum degree of G, which is at most the number of vertices K), and

$$\begin{aligned}
\gamma(H_B|_S) &= \gamma\left(\sum_{w=1}^{N} (A(G) - \mu(G))^{(w)}\big|_{\mathcal{W}_N(G)} \right) \\
&= \gamma\left((O_G - N\mu(G))\big|_{\mathrm{Wt}_N(G)} \right) \\
&= \theta_N(G) - N\mu(G).
\end{aligned}$$

Now applying the Lemma, we get

$$\lambda_N^1(G) = \gamma(H(G,N)) \geq \frac{2(\theta_N(G) - N\mu(G))}{2 + (\theta_N(G) - N\mu(G)) + 2K^2}.$$

Rearranging this inequality gives

$$\theta_N(G) - N\mu(G) \leq \lambda_N^1(G)\frac{2(K^2+1)}{2-\lambda_N^1(G)} \leq 4K^2\lambda_N^1(G) \leq 4K^2\epsilon^3$$

where in going from the second to the third inequality we used the fact that $1 \leq K^2$ in the numerator and $\lambda_N^1(G) \leq \epsilon^3 < 1$ in the denominator. Now using the fact (from the definition of Frustration-Free Bose-Hubbard Hamiltonian) that $\epsilon \leq \frac{1}{4K}$, we get

$$\theta_N(G) \leq N\mu(G) + \frac{\epsilon}{4},$$

i.e., the corresponding instance of XY Hamiltonian is a yes instance. $\square$

Chapter 9

Conclusions

There will definitely need to be some addition things here.

9.1 Open Problems

Heisenberg Modeaoeu

More simple graphs.

Is the constant term actually necessary?

References

[1] Andrew M. Childs and David Gosset. Levinson's theorem for graphs ii. *Journal of Mathematical Physics*, 53(10), 2012.

[2] Andrew M. Childs, David Gosset, and Zak Webb. Universal computation by multiparticle quantum walk. *Science*, 339(6121):791–794, 2013.

[3] Christophe Texier and Gilles Montambaux. Scattering theory on graphs. *Journal of Physics A: Mathematical and General*, 34(47):10307, 2001.