The computational power of many-body systems

by

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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.

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Chapter 1

Introduction

Well, I'd like to see where this goes.

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.

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.

1.5 Notation and requisite mathematics

I'm realizing that I'll need to include some information about graphs, positive-semidefinite matrices, etc. This will probably be the section on necessary terminology and mathematics, but I'm not sure what will go in here.

Lemma 1 (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*

$$\gamma\big(H_B|_S\big) \geq c > 0 \qquad \textit{and} \qquad \gamma(H_A) \geq d > 0. \tag{1.1}$$

Then,

$$\gamma(H_A + H_B) \geq \frac{cd}{d + \|H_B\|}. \tag{1.2}$$

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

$$\langle\psi|H_A + H_B|\psi\rangle = \gamma(H_A + H_B). \tag{1.3}$$

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

$$\langle\psi|H_A + H_B|\psi\rangle \geq \langle\psi|H_A|\psi\rangle \geq \gamma(H_A) \tag{1.4}$$

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

$$|\psi\rangle = \alpha|a\rangle + \beta|a^\perp\rangle \tag{1.5}$$

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

$$|f(q,r)\rangle = q|a\rangle + r|a^\perp\rangle \tag{1.6}$$

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

$$\gamma(H_A + H_B) = \min_{|q|^2+|r|^2=1} \langle f(q,r)|H_A + H_B|f(q,r)\rangle. \tag{1.7}$$

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

$$H_A|_Q = \begin{pmatrix} w & v^* \\ v & z \end{pmatrix} \qquad H_B|_Q = \begin{pmatrix} 0 & 0 \\ 0 & y \end{pmatrix} \tag{1.8}$$

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

$$M = H_A|_Q + H_B|_Q = \begin{pmatrix} w & v^* \\ v & y+z \end{pmatrix}. \tag{1.9}$$

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

$$\epsilon_+ = \|M\| \leq \|H_A|_Q\| + \|H_B|_Q\| \leq y + \|H_B|_Q\| \leq y + \|H_B\|, \tag{1.10}$$

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

$$\epsilon_+\epsilon_- = \det(M) = w(y+z) - |v|^2 \geq wy \tag{1.11}$$

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

$$\gamma(H_A + H_B) = \min_{|q|^2+|r|^2=1} \langle f(q,r)|H_A + H_B|f(q,r)\rangle = \epsilon_- \geq \frac{wy}{y + \|H_B\|}. \tag{1.12}$$

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

$$\gamma(H_A + H_B) \geq \frac{cd}{d + \|H_B\|} \tag{1.13}$$

as required. $\square$

1.6 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

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.

2.1 Introduction and 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

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

which requires the (unnormalizable) solutions,

$$\psi(x) = \exp(-ikx)$$

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

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

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.

2.1.1 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 Hilbert space of such a system corresponds to $n \in \mathbb{N}$, with the discretized second derivative taking the form

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

If we then rescale the energy levels, we have that the second ????

Altogether, we end up with the equation

$$\left(\sum_{x=-\infty}^{\infty} |\,x+1\rangle\langle x\,| + |\,x\rangle\langle x+1\,|\right)|\,\psi\,\rangle = E_\psi|\,\psi\,\rangle. \tag{2.1}$$

We can then break this vector equation into an equation for each basis vector $|\,x\,\rangle$, to get

$$\langle\,x+1\,|\,\psi\,\rangle + \langle\,x-1\,|\,\psi\,\rangle = E_\psi\langle\,x\,|\,\psi\,\rangle. \tag{2.2}$$

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

$$\langle\,x+1\,|\,\psi\,\rangle + \langle\,x-1\,|\,\psi\,\rangle = e^{ik}e^{ikx} + e^{-ik}e^{ikx} = E_\psi e^{ikx} = E_\psi\langle\,x\,|\,\psi\,\rangle \qquad \Rightarrow \qquad E_\psi = e^{ik} + e^{-ik} = 2\cos(k). \tag{2.3}$$

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 $[-\pi, \pi)$.

Now show how these form a basis for the states.

Hence, in analogy with the continuous case, our basis of states corresponds to momentum states, but where the possible momenta only range over $[-\pi, \pi)$. (As an aside, this maximum momenta is commonly know as a Leib-Robinson bound, and corresponds to a maximum speed of information propagation.)

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

$$s = \left|\frac{dE_k}{dk}\right| = 2\sin(|k|). \tag{2.4}$$

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.

2.2 Scattering off of a graph

Now that we have an example based on a free particle, we should examine how to generalize potentials. One method to do this is to add a potential function, with explicit potential energies at various vertices of the infinite path, but if we wish to only examine scattering on unweighted graphs, we need to be a little more clever. The interesting way to do this is to take a finite graph $\hat{G}$, and attach two semi-infinite paths to this graph. In this way, we get something that is similar to a finite-range potential.

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.

2.2.1 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. With this, the adjacency matrix of the graph G is then

$$A(G) = A(\widetilde{G}) + \sum_{v \in S \subset V(\widetilde{G})} |\,v\,\rangle\langle\,0\,| + |\,0\,\rangle\langle\,v\,| + \sum_{x=-\infty}^{\infty} |\,x\,\rangle\langle\,x+1\,| + |\,x+1\,\rangle\langle\,x\,|. \tag{2.5}$$

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

$$\langle\,x\,|\,\psi\,\rangle = \begin{cases} A_k e^{ikx} + B_k e^{ikx} & x \leq 0 \\ C_k e^{ikx} + D_k e^{ikx} & x \geq 0 \end{cases} \tag{2.6}$$

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

$$A(G)|\,\phi\,\rangle + (A_k + B_k) \sum_{v \in S} |\,v\,\rangle\langle\,v\,|\,\phi\,\rangle = 2\cos(k)|\,\phi\,\rangle, \tag{2.7}$$

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

$$2\cos(k)\langle 0 \,|\, \psi\rangle = Ae^{-ik} + B_k e^{ik} + C_k e^{ik} + D_k e^{-ik} + \sum_{v\in S}\langle v \,|\, \phi\rangle, \tag{2.8}$$

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

$$\langle x \,|\, \psi\rangle = \begin{cases} e^{-ikx} + B_k e^{ikx} & x \le 0 \\ C_k e^{-ikx} & x \ge 0 \end{cases} \tag{2.9}$$

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.

2.2.2 General graphs

More concretely, let $\widehat{G}$ be any finite graph, with $n+m$ vertices and an adjacency matrix

$$A(\widehat{G}) = \begin{pmatrix} A & B^\dagger \\ B & D \end{pmatrix}, \tag{2.10}$$

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. If each semi-infinite path is labeled as (x, i), where $x \ge 2$ is an integer and $i \in [N]$, then the adjacency matrix for G will be

$$A(G) = A(\widehat{G}) + \sum_{j=1}^{N}\sum_{x=1}^{\infty}\big(|\,x, j\,\rangle\langle\, x+1, j\,| + |\,x+1, j\,\rangle\langle\, x, j\,|\big). \tag{2.11}$$

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 forms of the state on the infinite path. We can easily see that the eigenstates along the path must have amplitude of the form $e^{\kappa x}$ for some κ, but the form of the κ determines these form.

2.2.2.1 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 $\widehat{G}$. In particular, we have that these states are eigenstates of the matrix D, with the further restriction that they are in the null space of the matrix $B^\dagger$.

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.

2.2.2.2 Unconfined bound states

The next interesting states are those that are not confined to the finite graph $\widehat{G}$, and thus they must take the form e^{ikx} along the semi-infinite paths. However, as we assume that the state is normalizable, we have to assume that $k \notin \mathbb{R}$, and further that $\Im(k) < 0$.

With this assumption, we have that the amplitudes along the paths decay exponentially, so that the state is bound to the graph $\widehat{G}$.

Note that the energy of the eigenstate is given by

$$E = e^{ik} + e^{-ik} \tag{2.12}$$

and as E must be real, we have that $k = i\kappa + n\pi$ for $\kappa < 0$. We can assume that n is either 0 or 1, as well.

[**TO DO:** *Finish this section, and figure out what values of κ are possible*]

[**TO DO:** *Are there only finitely many such κ, or is there a range of values?*]

2.2.2.3 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 $(\pm 1)^x$. I don't really know much about them.

[**TO DO:** *Finish this section, make it important*]

2.2.2.4 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 state corresponding to sending a particle in along one of the semi-infinite paths. Namely, we will assume that one of the paths has a portion of its amplitude 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

$$\langle x, q \,|\, \mathrm{sc}_j(k) \rangle = \delta_{j,q} e^{ikx} + S_{qj} e^{ikx}. \tag{2.13}$$

We then need to see whether such an eigenstate exists.

In particular, if we assume that such an eigenstate exists, and that [**TO DO:** *Finish this section*]

2.2.3 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

$$S(k) = -Q(z)^{-1}Q(z^{-1}), \tag{2.14}$$

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

$$Q(z) = \mathbb{I} - z\Big(A + B^\dagger \frac{1}{\frac{1}{z} + z - D} B\Big). \tag{2.15}$$

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

$$S(k)^\dagger = -Q(z^{-1})^\dagger (Q(z)^{-1})^\dagger \tag{2.16}$$

and that

$$Q(z)^\dagger = \mathbb{I}^\dagger - z^\dagger\Big(A^\dagger + B^\dagger\Big(\frac{1}{\frac{1}{z} + z - D}\Big)^\dagger (B^\dagger)^\dagger\Big) = \mathbb{I} - z^\dagger\Big(A + B^\dagger \frac{1}{\frac{1}{z^\dagger} + z^\dagger - D} B\Big) = Q(z^\dagger) \tag{2.17}$$

and thus

$$S(k)^\dagger = -Q(z^{-1})^\dagger (Q(z)^{-1})^\dagger = -Q(z)Q(z^{-1})^{-1} = Q(z^{-1})^{-1}Q(z) = S(k)^{-1} \tag{2.18}$$

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

$$S(k)^T = -\big(Q(z)^{-1}Q(z^{-1})\big)^T = -Q(z^{-1})^T (Q(z)^{-1})^T \tag{2.19}$$

$$= -Q(z^{-1})Q(z)^{-1} = -Q(z)^{-1}Q(z^{-1}) = S(k) \tag{2.20}$$

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.

2.2.4 Orthonormality of the scattering states

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 $i, j \in \{1, \ldots, N\}$,

$$\langle \mathrm{sc}_i(p)|\mathrm{sc}_j(k)\rangle = \langle \mathrm{sc}_i(p)|\Pi_1 + \Pi_2 - \Pi_3|\mathrm{sc}_j(k)\rangle = 2\pi\delta_{ij}\delta(k-p). \tag{2.21}$$

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

$$\begin{aligned}
\langle \mathrm{sc}_i(p)|\Pi_1|\mathrm{sc}_j(k)\rangle = 2\pi\delta_{ij}\delta(p-k) &+ \delta_{ij}\left(\frac{i}{2}\cot\left(\frac{p-k}{2}\right) - \frac{1}{2}\right) \\
&+ \sum_{q=1}^{N} S_{qi}^*(p)S_{qj}(k)\left(-\frac{i}{2}\cot\left(\frac{p-k}{2}\right) - \frac{1}{2}\right) \\
&+ S_{ji}^*(p)\left(-\frac{1}{2} - \frac{i}{2}\cot\left(\frac{p+k}{2}\right)\right) \\
&+ S_{ij}(k)\left(-\frac{1}{2} + \frac{i}{2}\cot\left(\frac{p+k}{2}\right)\right)
\end{aligned} \tag{2.22}$$

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

$$\begin{aligned}\langle \mathrm{sc}_i(p)|\Pi_2 - \Pi_3|\mathrm{sc}_j(k)\rangle &= \delta_{ij}\left(\frac{e^{2ip-ik} - e^{-2ik+ip}}{2\cos(p) - 2\cos(k)} - e^{ip-ik}\right) \\ &+ S^*_{ji}(p)\left(\frac{e^{-2ip-ik} - e^{-2ik-ip}}{2\cos(p) - 2\cos(k)} - e^{-ip-ik}\right) \\ &+ S_{ij}(k)\left(\frac{e^{2ip+ik} - e^{2ik+ip}}{2\cos(p) - 2\cos(k)} - e^{ip+ik}\right) \\ &+ \sum_{q=1}^{N} S^*_{qi}(p)S_{qj}(k)\left(\frac{e^{-2ip+ik} - e^{2ik-ip}}{2\cos(p) - 2\cos(k)} - e^{-ip+ik}\right) \\ &= \delta_{ij}\left(\frac{1}{2} - \frac{i}{2}\cot\left(\frac{p-k}{2}\right)\right) + S^*_{ji}(p)\left(\frac{1}{2} + \frac{i}{2}\cot\left(\frac{p+k}{2}\right)\right) \\ &+ S_{ij}(k)\left(\frac{1}{2} - \frac{i}{2}\cot\left(\frac{p+k}{2}\right)\right) \\ &+ \sum_{q=1}^{N} S^*_{qi}(p)S_{qj}(k)\left(\frac{1}{2} + \frac{i}{2}\cot\left(\frac{p-k}{2}\right)\right). \qquad (2.23)\end{aligned}$$

Adding equation (2.22) to equation (2.23) gives equation (2.21).

[**TO DO:** *Do they span the space of states, if you also include the bound states?*]

2.3 Applications of graph scattering

2.3.1 NAND Trees

[**TO DO:** *I need to give an explanation of this*]

2.3.2 Momentum dependent actions

While the NAND trees gives a good example of how the process works, we can generalize the idea to work at momenta other than [**TO DO:** *what momenta*] . In particular, we can attempt to find graph gadgets such that the scattering behaviour at some particular momenta is fixed.

2.3.2.1 R/T gadets

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.

2.3.2.2 Momentum Switches

We can generalize this idea of complete reflection or transmission to something called a momentum switch, in that with three inputs/outputs, for some chosen semi-infinite path, all incoming wavepackets at some momenta completely transmit to a second path, while all incoming wavepackets at some other particular momenta transmit to the third.

2.3.3 Encoded unitary

4 input/output, must go from in to out.

This is as very particular behavior.

2.4 Construction of graphs with particular scattering behavior

Note that while these scattering behaviors at particular momenta are easy to calculate, no efficient way currently exists to find a graph with a given scattering matrix, or even to tell whether or not such a graph exists. However, there are some special types of graphs that allow us to do this.

2.4.1 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 2. *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*

$$\sum_{i=1}^{n} \langle p_i|\chi_k\rangle \neq 0. \tag{2.24}$$

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 (2.24), 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 3. *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 $i \in [n]$,*

$$\sum_{\substack{v \in V(g_0): \\ (v,p_i) \in E(G_0)}} \langle v|\xi_k\rangle = c \neq 0 \tag{2.25}$$

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 (2.25), define a scattering state $|\psi_k\rangle$ on the full graph G, with amplitudes $\langle a|\psi_k\rangle = 1$,

$$\langle v|\psi_k\rangle = \begin{cases} -\frac{1}{c}\langle v|\xi_k\rangle & v \in V(g_0) \\ 0 & v \in P \end{cases} \tag{2.26}$$

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 2, 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 (2.26) 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. $\square$

2.4.2 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 4. *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 3 shows that the graph g_0 has a $2\cos(k)$-eigenvector $|\xi_k\rangle$ satisfying equation (2.25) 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 2 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 $\mathcal{T}$. □

2.4.3 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*]

In particular, we have that these graphs have nice scattering behaviors, and will be useful in the long run.

Additionally, it is possible to combine some graphs in a manner that can be used

2.5 Various facts about scattering

These are facts that will be of use to us.

2.5.1 Degree-3 graphs are sufficent

Replace each vertex by a path of fixed length. I should turn this into a lemma.

Lemma 5. *Let $\widehat{G}$ be a finite graph, and let M be a finite set of rational multiples of π. There exists a degree 3 graph $\widehat{H}$ such that the scattering matrix arising from $\widehat{H}$ is equal to the scattering matrix arising from $\widehat{G}$ for each $ki \in M$.*

Proof. The graph $\widehat{H}$ is constructed from $\widehat{G}$ by replacing each vertex with large degree by a path of some length related to the momenta in M. If the path is taken to be the correct size, by inspecting the resulting eigenvectors we can show that the scattering amplitudes of the new graph are equal to the scattering graphs of the old graph.

In particular, let $\widehat{G}$ be as described, and let $w \in V(G)$ be any vertex of degree $d > 3$. Additionally, let L be the least integer such that $Lk/\pi \in \mathbb{Z}$ for each $k \in M$ (i.e., the least common multiple of the denominators of each $k \in M$). Let $\widetilde{H}$ be the graph obtained by

[**TO DO:** *Finish this proof*] □

2.5.2 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*]

2.5.2.1 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

$$|\tau_k\rangle = (H \pm \sqrt{2}\mathbb{I})|w_k\rangle. \tag{2.27}$$

2.5.2.2 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 $T = 0$. □

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 2.5.2.1, 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 (2.27). This gives

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

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 $x \geq 0$,

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

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

$$\alpha(H + \sqrt{2}\mathbb{I})|c\rangle = \alpha(H + \sqrt{2}\mathbb{I})|a\rangle + \beta(H + \sqrt{2}\mathbb{I})|b\rangle = |{}_1(-\tfrac{\pi}{4})\rangle, \tag{2.28}$$

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 $p = -\frac{5\pi}{6}$.

Chapter 3

Universality of single-particle scattering

3.1 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*

$$|\psi^j(0)\rangle = \frac{1}{\sqrt{L}} \sum_{x=M+1}^{M4L} e^{-ikx} |x, j\rangle. \tag{3.1}$$

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

$$\left\| e^{-iH_G t} |\psi^j(0)\rangle - |\alpha^j(t)\rangle \right\| = \mathcal{O}(L^{-1/4}) \tag{3.2}$$

where

$$|\alpha^j(t)\rangle = \frac{1}{\sqrt{L}} e^{-2it\cos k} \sum_{x=1}^{\infty} \sum_{q=1}^{N} (\delta_{qj} e^{-ikx} R(x - \lfloor 2t \sin k \rfloor) + S_{qj}(k) e^{ikx} R(-x - \lfloor 2t \sin k \rfloor)) |x, q\rangle \tag{3.3}$$

with

$$R(l) = \begin{cases} 1 & \text{if } l - M \in [L] \\ 0 & \text{otherwise.} \end{cases} \tag{3.4}$$

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:

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

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

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

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

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

where

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

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 $|\,\psi^j(t)\,\rangle \approx |\,w^j(t)\,\rangle \approx |\,w^j_A(t)\,\rangle \approx |\,\alpha^j(t)\,\rangle$.

Now

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

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

$$\begin{aligned}
\frac{1}{L}\left(\int_{\epsilon}^{\pi} + \int_{-\pi}^{-\epsilon}\right) \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)} &= \frac{2}{L} \int_{\epsilon}^{\pi} \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)} \\
&\leq \frac{2}{L} \int_{\epsilon}^{\pi} \frac{d\phi}{2\pi} \frac{\pi^2}{\phi^2} \\
&\leq \frac{\pi}{L\epsilon}.
\end{aligned} \tag{3.5}$$

Therefore

$$1 \geq \langle w^j_A(t)|w^j_A(t)\rangle \geq 1 - \frac{\pi}{L\epsilon}.$$

Similarly,

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

and, using the unitarity of S,

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

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

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

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

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

Hence

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

so

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

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

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

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

$$\left\||w_A^j(t)\rangle - |\alpha^j(t)\rangle\right\| = \emptyset(L^{-1/8}). \tag{3.6}$$

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 (3.6) it is sufficient to show that

$$\left\| P|w_A^j(t)\rangle - |\alpha^j(t)\rangle \right\| = \emptyset(L^{-1/4}) \tag{3.7}$$

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

$$\begin{aligned}\left\| (1-P)\, |w_A^j(t)\rangle \right\|^2 &= \left\| |w_A^j(t)\rangle \right\|^2 - \left\| P|w_A^j(t)\rangle \right\|^2 \\ &\leq 1 - \left(1 + \emptyset(L^{-1/4})\right) \\ &= \emptyset(L^{-1/4}). \end{aligned} \tag{3.8}$$

From the above formula we now see that inequality (3.7) implies (3.6).

Noting that

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

we write

$$\begin{aligned}\langle x, q|\alpha^j(t)\rangle = e^{-2it\cos k} \Bigg(& \delta_{qj} e^{-ikx} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi(x - \lfloor 2t \sin k \rfloor)} f(\phi) \\ & + S_{qj}(k) e^{ikx} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi(-x - \lfloor 2t \sin k \rfloor)} f(\phi) \Bigg). \end{aligned} \tag{3.9}$$

On the other hand,

$$\langle x, q|w_A^j(t)\rangle = \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} e^{-2it\cos(k+\phi)} f(\phi) \left(e^{-i(k+\phi)x} \delta_{qj} + e^{i(k+\phi)x} S_{qj}(k+\phi) \right). \tag{3.10}$$

Using equations (3.9) and (3.10) 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:

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

where we have used the facts that $|e^{is}-1|^2 \leq s^2$ 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

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

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 (3.5) 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

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

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

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

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

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

3.2 Using scattering for simple computation

3.3 Encoded two-qubit gates

3.4 Single-qubit blocks

3.5 Combining blocks

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

Chapter 4

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.

4.1 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.

4.1.1 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

$$H^{(2)} = H_x^{(1)} \otimes \mathbb{I}_y + \mathbb{I}_x \otimes H_y^{(1)} + \sum_{x,y\in\mathbb{Z}} \mathcal{V}(|x-y|)\,|x, y\rangle\langle x, y| \tag{4.1}$$

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

$$H_s^{(1)} \otimes H_r^{(1)} + \mathbb{I}_s \otimes \sum_{r\in\mathbb{Z}} \mathcal{V}(|r|)\,|\, r\,\rangle\langle\, r\,|. \tag{4.2}$$

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

$$2\cos\left(\frac{p_1}{2}\right) H_r^{(1)} + \sum_{r\in\mathbb{Z}} \mathcal{V}(|r|)\,|\, r\,\rangle\langle\, r\,| \tag{4.3}$$

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

$$\langle r|\psi(p_1; p_2)\rangle = \begin{cases} e^{-ip_2 r} + R(p_1, p_2)e^{ip_2 r} & \text{if } r \le -C \\ f(p_1, p_2, r) & \text{if } |r| < C \\ T(p_1, p_2)e^{-ip_2 r} & \text{if } r \ge C \end{cases} \tag{4.4}$$

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

$$\langle\, s;r\,|\,\mathrm{sc}(p_1;p_2)\,\rangle_\pm = \frac{1}{\sqrt{2}}e^{-ip_1 s/2}\begin{cases} e^{-ip_2 r} \pm e^{i\theta_\pm(p_1,p_2)}e^{ip_2 r} & \text{if } r \le -C \\ f(p_1,p_2,r) \pm f(p_1,p_2,-r) & \text{if } |r| < C \\ e^{i\theta_\pm(p_1,p_2)}e^{-ip_2 r} \pm e^{ip_2 r} & \text{if } r \ge C \end{cases} \tag{4.5}$$

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

$$e^{i\theta_\pm(p_1,p_2)} = T(p_1,p_2) \pm R(p_1,p_2). \tag{4.6}$$

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 **??**).

4.1.2 Finite truncation

Theorem 2. *Let $H^{(2)}$ be a two-particle Hamiltonian of the form (4.1) 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 (4.6). Define $\theta = \theta_\pm(\pi/4, 3\pi/8)$. Let $L \in \mathbb{N}^+$, let $M \in \{C+1, C+2, \dots\}$, 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 $0 \le t \le c_0 L$, we have

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

where

$$|\alpha(t)\rangle = \sum_{x,y} a_{xy}(t)|x,y\rangle, \tag{4.7}$$

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

$$a_{xy}(t) = \frac{1}{\sqrt{2}L} e^{-\sqrt{2}it} \left[e^{-i\pi x/2} e^{i\pi y/4} F(x,y,t) \pm e^{i\theta} e^{i\pi x/4} e^{-i\pi y/2} F(y,x,t) \right] \tag{4.8}$$

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 4.1.2.1. The proof follows the method used in the single-particle case, which is based on the calculation from the appendix of reference [**?**].

Recall from (4.5) that for each $p_1 \in (-\pi, \pi)$ and $p_2 \in (0, \pi)$ there is an eigenstate $|\text{sc}(p_1; p_2)\rangle_\pm$ of $H^{(2)}$ of the form

$$\langle x,y|\text{sc}(p_1;p_2)\rangle_\pm = \frac{e^{-ip_1\left(\frac{x+y}{2}\right)}}{\sqrt{2}} \begin{cases} e^{-ip_2(x-y)} \pm e^{i\theta_\pm(p_1,p_2)} e^{ip_2(x-y)} & \text{if } x - y \leq -C \\ e^{-ip_2(x-y)} e^{i\theta_\pm(p_1,p_2)} \pm e^{ip_2(x-y)} & \text{if } x - y \geq C \\ f(p_1,p_2,x-y) \pm f(p_1,p_2,y-x) & \text{if } |x-y| < C \end{cases} \tag{4.9}$$

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 $|\text{sc}(p_1;p_2)\rangle_\pm$ satisfies

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

and is delta-function normalized as

$${}_\pm\langle \text{sc}(p_1';p_2')|\text{sc}(p_1;p_2)\rangle_\pm = 4\pi^2 \delta(p_1 - p_1')\delta(p_2 - p_2'). \tag{4.10}$$

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

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

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 (4.9) we get

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

where

$$|\psi_A(t)\rangle = \iint_{D_\epsilon} \frac{d\phi_1 d\phi_2}{4\pi^2} e^{-it4\cos(\frac{\pi}{8}+\frac{\phi_1}{2})\cos(\frac{3\pi}{8}+\phi_2)} A(\phi_1, \phi_2) |\mathrm{sc}(\tfrac{\pi}{4}+\phi_1; \tfrac{3\pi}{8}+\phi_2)\rangle_\pm \tag{4.11}$$

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

with

$$A(\phi_1, \phi_2) = \frac{1}{L} \sum_{x=-(M+L)}^{-(M+1)} \sum_{y=M+1}^{M+L} e^{i\phi_1 \frac{x+y}{2}} e^{i\phi_2(x-y)} \tag{4.12}$$

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

Using the delta-function normalization of the scattering states (equation (4.10)) 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 8 (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 8) 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

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

Now

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

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 6. *With $|\psi_A(t)\rangle$ and $|\alpha(t)\rangle$ defined through equations (4.11) and (4.7), with $t \le c_0 L$ (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

$$\| \, |\psi_A(t)\rangle - |\alpha(t)\rangle \| \le 2 \, \|P_1|\psi_A(t)\rangle - P_1|\alpha(t)\rangle\| + \|P_2|\,\psi_A(t)\,\rangle\| + \|P_2|\,\alpha(t)\,\rangle\| \, ,$$

where

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

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

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

From Lemma 9, for $x \le y$, the state $|\,\alpha(t)\,\rangle$ takes the form

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

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 $y - x \ge C$)

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

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

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

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

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

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

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

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

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

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

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

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

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

where we have used Lemma 8 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

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

by Lemma 8, and similarly

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

Moving on to the next term,

$$\begin{aligned}\langle g_1(t)|g_1(t)\rangle \le \frac{1}{2}\iint_{D_\epsilon}\frac{d\phi_1 d\phi_2}{4\pi^2}\left|A(\phi_1,\phi_2)\right|^2 \Big| & e^{-it4\cos\left(\frac{\pi}{8}+\frac{\phi_1}{2}\right)\cos\left(\frac{3\pi}{8}+\phi_2\right)} \\ & - e^{-it\left(\sqrt{2}+\sqrt{2}\left(\frac{\phi_1}{2}-\phi_2\right)-2\left(\frac{\phi_1}{2}+\phi_2\right)\right)}\Big|^2 \\ \le \frac{1}{2}\iint_{D_\epsilon}\frac{d\phi_1 d\phi_2}{4\pi^2}\Bigg[& \left|A(\phi_1,\phi_2)\right|^2 t^2\left(4\cos\left(\frac{\pi}{8}+\frac{\phi_1}{2}\right)\cos\left(\frac{3\pi}{8}+\phi_2\right)\right. \\ & \left.-\sqrt{2}-\sqrt{2}\left(\frac{\phi_1}{2}-\phi_2\right)+2\left(\frac{\phi_1}{2}+\phi_2\right)\right)^2\Bigg]\end{aligned}\tag{4.13}$$

using $\left|e^{-ic}-1\right|^2 \le c^2$ 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

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

using $|\cos x - 1| \leq x^2$ and $|\sin x - x| \leq x^2$ for $x \in \mathbb{R}$. Plugging this into equation (4.13) 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 (4.17) 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 (4.3). 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 $\theta = \theta_\pm(\pi/4, 3\pi/8)$,

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

for some constant Γ (independent of L). Therefore

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

Putting these bounds together, we get

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

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

$$\| P_1 |\psi_A(t)\rangle - P_1 |\alpha(t)\rangle \| = \mathcal{O}(L^{-1/4}). \tag{4.14}$$

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

$$\| P_2 |\, \alpha(t) \,\rangle \| = \mathcal{O}(L^{-1/2}). \tag{4.15}$$

We now use the bounds (4.14) and (4.15) and Lemma 7 to show that

$$\| |\psi_A(t)\rangle - |\alpha(t)\rangle \| = \mathcal{O}(L^{-1/8}). \tag{4.16}$$

First consider the case where the interaction range is $C = 0$ (as in the Bose-Hubbard model). In this case equation (4.16) follows directly from equation (4.14) 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 $C \neq 0$. In this case

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

where in the next-to-last line we have used Lemma 7. So

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

which completes the proof. □

□

4.1.2.1 Technical lemmas

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

Lemma 7. *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

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

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

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

Letting

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

we have

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

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

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

since $l<L$. ∎

Lemma 8. *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 (4.12).

Proof. Using equation (4.12) 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 (4.12) we get

$$|A(\phi_1,\phi_2)|^2 = \frac{1}{L^2}\frac{\sin^2(\frac{1}{2}L[\frac{\phi_1}{2}+\phi_2])}{\sin^2(\frac{1}{2}[\frac{\phi_1}{2}+\phi_2])}\frac{\sin^2(\frac{1}{2}L[\frac{\phi_1}{2}-\phi_2])}{\sin^2(\frac{1}{2}[\frac{\phi_1}{2}-\phi_2])}. \tag{4.17}$$

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

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

Proof. The lemma follows from (4.8) 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. □

4.2 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.

4.2.1 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

$$S_{\text{switch}}(-\pi/4) = \begin{pmatrix} 0 & 0 & e^{-i\pi/4} \\ 0 & -1 & 0 \\ e^{-i\pi/4} & 0 & 0 \end{pmatrix} \qquad S_{\text{switch}}(-\pi/2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}. \tag{4.18}$$

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 $|1_{\text{in}}\rangle^{\mathrm{m}}$, 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

$$Z = 4L \tag{4.19}$$
$$X = d_2 + L + M\left(-\frac{\pi}{2}\right) \tag{4.20}$$
$$W = d_1 + L + M\left(-\frac{\pi}{4}\right) \tag{4.21}$$

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,

$$\left\| e^{-iH^{(2)}_{G'}t_{\rm II}}|00_{\rm in}\rangle^{c,\rm m} - |00_{\rm out}\rangle^{c,\rm m} \right\| = \emptyset(L^{-1/4}) \tag{4.22}$$

$$\left\| e^{-iH^{(2)}_{G'}t_{\rm II}}|01_{\rm in}\rangle^{c,\rm m} - |01_{\rm out}\rangle^{c,\rm m} \right\| = \emptyset(L^{-1/4}) \tag{4.23}$$

$$\left\| e^{-iH^{(2)}_{G'}t_{\rm II}}|10_{\rm in}\rangle^{c,\rm m} - |10_{\rm out}\rangle^{c,\rm m} \right\| = \emptyset(L^{-1/4}) \tag{4.24}$$

$$\left\| e^{-iH^{(2)}_{G'}t_{\rm II}}|11_{\rm in}\rangle^{c,\rm m} - e^{i\theta}|11_{\rm out}\rangle^{c,\rm m} \right\| = \emptyset(L^{-1/4}) \tag{4.25}$$

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

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

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

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

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 (4.22), (4.23), and (4.24) 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 $|00_{\rm in}\rangle^{c,\rm m}$, 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 $|0_{\rm in}\rangle^{c}$ and evolving for time $t_{\rm II}$ with the single-particle Hamiltonian for the top path, we obtain the final state

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

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

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

Putting these bounds together we get the bound (4.22).

In the case where the input state is $|10_{\rm in}\rangle^{c,\rm m}$ (or $|01_{\rm in}\rangle^{c,\rm m}$) 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 (4.18). 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 (4.24) 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

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

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 $\mathcal{O}(L^{-1/4})$, 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 $\mathcal{O}(L^{-1/4})$, establishing (4.24). For the bound (4.23), 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 $\mathcal{O}(L^{-1/4})$. 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 $\mathcal{O}(L^{-1/4})$). 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 $\delta = \mathcal{O}(L^{-1/4})$. 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

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

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 $\mathcal{O}(L^{-1/4})$) 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 $\mathcal{O}(L^{-1/4})$). Using $H^{(2)}_{G_B}$ (rather than $H^{(2)}_{G'}$) to evolve the state on this interval, we incur errors bounded as $\mathcal{O}(L^{-1/4})$ (using the truncation lemma with $N_0 = \Theta(L)$, $W = \tilde{H} = H^{(2)}_{G_B}$, $H = H^{(2)}_{G'}$, and $\delta = \mathcal{O}(L^{-1/4})$).

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 $\text{Ø}(L^{-1/4})$. This establishes equation (4.25). In Figure **??** we illustrate the movement of the two wave packets through the graph when the initial state is $|11_{\mathrm{in}}\rangle^{c,\mathrm{m}}$.

4.3 Universal Computation

4.3.1 Two-qubit blocks

4.3.2 Combining blocks

4.4 Improvements and Modifications

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

Chapter 5

Ground energy of quantum walk

To get some flavor for QMA-completeness results.

5.1 Encoding computations as states

5.1.1 History states

5.2 Determining ground energy of a sparse adjacency matrix is QMA-complete

5.2.1 Kitaev Hamiltonian

5.2.2 Transformation to Adjacency Matrix

We suppose $\mathcal{C}_x$ implements a unitary

$$U_{\mathcal{C}_x} = U_M \dots U_2 U_1 \tag{5.1}$$

where each U_i is from the universal gate set

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

with

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \quad T = \begin{pmatrix}1 & 0\\ 0 & e^{i\frac{\pi}{4}}\end{pmatrix} \quad \text{CNOT} = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}.$$

The verification circuit $\mathcal{C}_x$ has an n_{input}-qubit input register and $n - n_{\text{input}}$ ancilla qubits initialized to $|0\rangle$ at the beginning of the computation. One of these n qubits serves as an output qubit.

It will be convenient to consider

$$U^\dagger_{\mathcal{C}_x} U_{\mathcal{C}_x} = W_{2M} \dots W_2 W_1$$

where

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

As in Section **??** we start with a version of the Feynman-Kitaev Hamiltonian [**?**, **?**]

$$H_x = -\sqrt{2} \sum_{t=1}^{2M} \left(W_t^{\dagger} \otimes |t\rangle\langle t+1| + W_t \otimes |t+1\rangle\langle t| \right) \tag{5.2}$$

acting on the Hilbert space $\mathcal{H}_{\text{comp}} \otimes \mathcal{H}_{\text{clock}}$ where $\mathcal{H}_{\text{comp}} = (\mathbb{C}^2)^{\otimes n}$ is an n-qubit computational register and $\mathcal{H}_{\text{clock}} = \mathbb{C}^{2M}$ is a $2M$-level register with periodic boundary conditions (i.e., we let $|2M+1\rangle = |1\rangle$). Note that

$$V^{\dagger} H_x V = -\sqrt{2} \sum_{t=1}^{2M} \left(\mathbb{I} \otimes |t\rangle\langle t+1| + \mathbb{I} \otimes |t+1\rangle\langle t| \right) \tag{5.3}$$

where

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

and $W_0 = 1$. Since V is unitary, the eigenvalues of H_x are the same as the eigenvalues of (5.3), namely

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

for $\ell = 0, \ldots, 2M-1$. The ground energy of (5.3) is $-2\sqrt{2}$ and its ground space is spanned by

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

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

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

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

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

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

$$\eta + 2\sqrt{2} \geq \sqrt{2} \frac{\pi^2}{M^2} \tag{5.4}$$

(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_x are also integer powers of $\omega = e^{i\frac{\pi}{4}}$. We consider the 8×8 shift operator

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

and note that ω is an eigenvalue of S with eigenvector

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

We modify H_x as follows. For each operator $-\sqrt{2}H$, $-\sqrt{2}HT$, $-\sqrt{2}(HT)^{\dagger}$, or $-\sqrt{2}\,(H \otimes \mathbb{I})\,\mathrm{CNOT}$ appearing in equation (5.2), 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 (6.2) gives

$$H_{\mathrm{prop}} = \sum_{t=1}^{2M} \left(B(W_t)_{13}^{\dagger} \otimes |t\rangle\langle t+1|_2 + B(W_t)_{13} \otimes |t+1\rangle\langle t|_2 \right) \tag{5.5}$$

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_x that we started with (see equation (5.2)). There is also a sector (where S has eigenvalue ω^*) where the Hamiltonian is the complex conjugate of H_x. 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 (5.5) 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 $\|H_{\mathrm{prop}}\| \leq 4$, 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

$$\mathcal{H}_{\mathrm{comp}} \otimes \mathcal{H}_{\mathrm{clock}} \otimes \mathcal{H}_{\mathrm{anc}}$$

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

$$A_x = H_{\text{prop}} + H_{\text{penalty}} + H_{\text{input}} + H_{\text{output}} \tag{5.6}$$

where

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

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 (5.6). 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

$$e_1 = -2\sqrt{2} + \left(-1 - \sqrt{2}\right) = -1 - 3\sqrt{2} = -5.24\ldots, \tag{5.7}$$

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

$$\frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} W_{t-1}W_{t-2}\ldots W_1|\phi\rangle|t\rangle|\omega\rangle \tag{5.8}$$
$$\frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} (W_{t-1}W_{t-2}\ldots W_1)^*|\phi^*\rangle|t\rangle|\omega^*\rangle \tag{5.9}$$

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

5.2.3 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

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

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 (5.8)). One can also directly verify that $|\text{wit}\rangle$ has zero energy for H_{input}. Thus

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

5.2.4 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

$$\gamma(H_{\text{prop}} + H_{\text{penalty}} - e_1 \cdot \mathbb{I}) \geq \min\left\{\sqrt{2}\frac{\pi^2}{M^2}, -5 - e_1\right\} \geq \frac{1}{5M^2}. \tag{5.10}$$

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 (5.4) on the energy gap of H_x.

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

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

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 (5.8) and (5.9) 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 (5.10), and clearly $\|H_B\| \leq n$. Thus Lemma **??** gives

$$\gamma(H_{\text{prop}} + H_{\text{penalty}} + H_{\text{input}} - e_1 \cdot \mathbb{I}) \geq \frac{\left(\frac{1}{5M^2}\right)\left(\frac{1}{2M}\right)}{\frac{1}{5M^2} + \frac{1}{2M} + n} \geq \frac{1}{10M^3\,(1+n)} \geq \frac{1}{20M^3 n}. \tag{5.11}$$

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

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

Let S_A be the ground space of H_A. Note that it is spanned by states of the form (5.8) and (5.9) 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

$$\frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} W_{t-1} W_{t-2} \dots W_1 \left(|\psi\rangle |0\rangle^{\otimes n - n_{\text{input}}} \right) |t\rangle |\omega\rangle \tag{5.12}$$

and another block for states of the form

$$\frac{1}{\sqrt{2M}} \sum_{t=1}^{2M} (W_{t-1} W_{t-2} \dots W_1)^* \left(|\psi\rangle^* |0\rangle^{\otimes n - n_{\text{input}}} \right) |t\rangle |\omega^*\rangle. \tag{5.13}$$

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 (5.12) for some state $|\psi\rangle$. Thus the minimum eigenvalue within this block is the minimum expectation of H_{output} in a state (5.12), where the minimum is taken over all n_{input}-qubit states $|\psi\rangle$. This is equal to

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

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 (5.13) for some state $|\psi\rangle$, and the minimum eigenvalue within this block is

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

(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

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

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 (5.11)), we get

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

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.

Chapter 6

Ground energy of multi-particle quantum walk

6.1 Introduction

6.1.1 Containment in QMA

6.1.2 Reduction to frustration-free case

6.2 Constructing the underlying graph for QMA-hardness

6.2.1 Gate graphs

In this Section we define a class of graphs (*gate graphs*) and a diagrammatic notation for them (*gate diagrams*). We also discuss the Bose-Hubbard model on these graphs.

Every gate graph is constructed using a specific 128-vertex graph g_0 as a building block. This graph is shown in Figure **??** 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.

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

$$e_1 = -1 - 3\sqrt{2}. \tag{6.1}$$

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.

6.2.1.1 The graph g_0

The graph g_0 shown in Figure **??** is closely related to a single-qubit circuit $\mathcal{C}_0$ with eight gates U_j for $j \in [8]$, where

$$U_1 = U_2 = U_7 = U_8 = H \qquad U_3 = U_5 = HT \qquad U_4 = U_6 = (HT)^\dagger$$

with

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}.$$

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.

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

$$-\sqrt{2}\sum_{t=1}^{8}\Big(U_t^\dagger \otimes |t\rangle\langle t+1| + U_t \otimes |t+1\rangle\langle t|\Big). \tag{6.2}$$

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 (6.2) 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 (6.2) 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 (6.2) 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 (6.2), 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 (6.2). This gives

$$H_{\text{prop}} = \sum_{t=1}^{8} \left(B(U_t)_{13}^{\dagger} \otimes |t\rangle\langle t+1|_2 + B(U_t)_{13} \otimes |t+1\rangle\langle t|_2 \right), \tag{6.3}$$

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 (6.2). 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

$$-2\sqrt{2} + (-1-\sqrt{2}) = -1 - 3\sqrt{2} = -5.24\ldots. \tag{6.4}$$

This is the constant e_1 from equation (6.1). 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

$$|\psi_{z,0}\rangle = \frac{1}{\sqrt{8}} \big(|z\rangle(|1\rangle + |3\rangle + |5\rangle + |7\rangle) + H|z\rangle(|2\rangle + |8\rangle) + HT|z\rangle(|4\rangle + |6\rangle) \big) |\omega\rangle \tag{6.5}$$

$$|\psi_{z,1}\rangle = |\psi_{z,0}\rangle^* \tag{6.6}$$

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 $|z\rangle$.

6.2.1.2 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 (6.5) 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

$$A(G) = \mathbb{I}_q \otimes A(g_0) + h_{\mathcal{S}} + h_{\mathcal{E}} \tag{6.7}$$

$$h_{\mathcal{S}} = \sum_{\mathcal{S}} |q,z,t\rangle\langle q,z,t| \otimes \mathbb{I}_j \tag{6.8}$$

$$h_{\mathcal{E}} = \sum_{\mathcal{E}} \left(|q,z,t\rangle + |q',z',t'\rangle\right)\left(\langle q,z,t| + \langle q',z',t'|\right) \otimes \mathbb{I}_j. \tag{6.9}$$

The sums in equations (6.8) and (6.9) 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 (6.8) and (6.9) are sums of orthogonal Hermitian operators. Therefore

$$\|h_{\mathcal{S}}\| = \max_{\mathcal{S}} \left\| |q,z,t\rangle\langle q,z,t| \otimes \mathbb{I}_j \right\| = 1 \quad \text{if } \mathcal{S} \neq \emptyset \tag{6.10}$$

$$\|h_{\mathcal{E}}\| = \max_{\mathcal{E}} \left\| \left(|q,z,t\rangle + |q',z',t'\rangle\right)\left(\langle q,z,t| + \langle q',z',t'|\right) \otimes \mathbb{I}_j \right\| = 2 \quad \text{if } \mathcal{E} \neq \emptyset \tag{6.11}$$

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*]

6.2.1.3 Frustration-free states for a given interaction range

Consider the adjacency matrix $A(G)$ of a gate graph G, and note (from equation (6.7) 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 1. 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

$$(\mathbb{I} \otimes A(g_0))\, |\Gamma\rangle = e_1 |\Gamma\rangle \tag{6.12}$$

$$h_{\mathcal{S}} |\Gamma\rangle = 0 \tag{6.13}$$

$$h_{\mathcal{E}} |\Gamma\rangle = 0. \tag{6.14}$$

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 (6.12) 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 (6.5) and (6.6). The coefficients in the superposition are then constrained by equations (6.13) and (6.14).

Example 1. As an example, we show the gate graph in Figure **??** is an e_1-gate graph. As noted above, equation (6.12) 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

$$\big(\tau_1|\psi^1_{0,a}\rangle + \nu_1|\psi^1_{1,a}\rangle\big) + \big(\tau_2|\psi^2_{0,a}\rangle + \nu_2|\psi^2_{1,a}\rangle\big)$$

and note that in this case (6.13) implies $\tau_1 = 0$. Equation (6.14) gives

$$\begin{pmatrix}\tau_2\\ \nu_2\end{pmatrix} = \begin{cases} HT\begin{pmatrix}-\tau_1\\ -\nu_1\end{pmatrix} & a = 0\\[2ex] (HT)^*\begin{pmatrix}-\tau_1\\ -\nu_1\end{pmatrix} & a = 1.\end{cases}$$

We find two orthogonal e_1-energy states, which are (up to normalization)

$$|\psi^1_{1,0}\rangle - \frac{e^{i\frac{\pi}{4}}}{\sqrt{2}}\left(|\psi^2_{0,0}\rangle - |\psi^2_{1,0}\rangle\right) \tag{6.15}$$

$$|\psi^1_{1,1}\rangle - \frac{e^{-i\frac{\pi}{4}}}{\sqrt{2}}\left(|\psi^2_{0,1}\rangle - |\psi^2_{1,1}\rangle\right). \tag{6.16}$$

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 10. $\lambda^1_2(g_0) > 0$.

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

$$(|v\rangle\langle v| \otimes |v\rangle\langle v|)\, |Q\rangle = 0 \tag{6.17}$$

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 (6.17) 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 (6.17) 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. $\square$

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:

$$\mathcal{I}(G, N) = \mathrm{span}\{\mathrm{Sym}(|\psi^{q_1}_{z_1,a_1}\rangle \ldots |\psi^{q_N}_{z_N,a_N}\rangle) \colon z_i, a_i \in \{0, 1\},\ q_i \in [R],\ q_i \neq q_j \text{ whenever } i \neq j\}. \tag{6.18}$$

Lemma 11. *Let G be an e_1-gate graph. A state $|\Gamma\rangle \in \mathcal{Z}_N(G)$ is frustration free if and only if*

$$(A(G) - e_1)^{(w)}\, |\Gamma\rangle = 0 \ \text{ for all } w \in [N] \tag{6.19}$$

$$|\Gamma\rangle \in \mathcal{I}(G, N). \tag{6.20}$$

Proof. First suppose that equations (6.19) and (6.20) hold. From (6.20) we see that $|\Gamma\rangle$ has no support on states where two or more particles are located at the same vertex. Hence

$$\sum_{k\in V} \hat{n}_k \left(\hat{n}_k - 1\right) |\Gamma\rangle = 0. \tag{6.21}$$

Putting together equations (6.19) and (6.21), we get

$$H(G,N)|\Gamma\rangle = \left(H_G^N - Ne_1\right)|\Gamma\rangle = 0,$$

so $|\Gamma\rangle$ is frustration free.

To complete the proof, we show that if $|\Gamma\rangle$ is frustration free, then conditions (6.19) and (6.20) hold. By definition, a frustration-free state $|\Gamma\rangle$ satisfies

$$H(G,N)|\Gamma\rangle = \left(\sum_{w=1}^{N} \left(A(G) - e_1\right)^{(w)} + \sum_{k\in V} \hat{n}_k \left(\hat{n}_k - 1\right)\right)|\Gamma\rangle = 0. \tag{6.22}$$

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 (6.19) 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 (6.22) also implies

$$H(G_{\text{rem}}, N)|\Gamma\rangle = 0. \tag{6.23}$$

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 **??** (along with knowledge of the eigenvalues and eigenvectors of g_0). By Lemma 10 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 (6.23) we get $|\Gamma\rangle \in \mathcal{I}(G,N)$. □

Note that if $\mathcal{I}(G,N)$ is empty then Lemma 11 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 11 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 (6.20) holds, then all k-particle reduced density matrices of $|\Gamma\rangle$ are contained in $\mathcal{I}(G, k)$. Furthermore, (6.19) 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.

6.2.2 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 (6.7), we write the adjacency matrix of the corresponding gate graph G_W as

$$A(G_W) = \sum_{q=1}^{6} |q\rangle\langle q| \otimes A(g_0) + h_{\mathcal{E}} \tag{6.24}$$

where $h_{\mathcal{E}}$ is given by (6.9) 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 (6.24) 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 (6.14) (in this case equation (6.13) is automatically satisfied since $h_{\mathcal{S}} = 0$). Enforcing (6.14) gives eight equations, one for each edge in the gate diagram:

$$\begin{aligned} \tau_3 &= -\tau_1 & \frac{1}{\sqrt{2}}(\tau_1 + \nu_1) &= -\tau_6 \\ \tau_4 &= -\nu_1 & \frac{1}{\sqrt{2}}(\tau_1 - \nu_1) &= -\tau_5 \\ \nu_3 &= -\tau_2 & \frac{1}{\sqrt{2}}(\tau_2 + \nu_2) &= -\nu_5 \\ \nu_4 &= -\nu_2 & \frac{1}{\sqrt{2}}(\tau_2 - \nu_2) &= -\nu_6. \end{aligned}$$

There are four linearly independent solutions to this set of equations, given by

Solution 1: $\tau_1 = 1 \quad \tau_3 = -1 \quad \tau_5 = -\frac{1}{\sqrt{2}} \quad \tau_6 = -\frac{1}{\sqrt{2}}$ all other coefficients 0

Solution 2: $\nu_1 = 1 \quad \tau_4 = -1 \quad \tau_5 = \frac{1}{\sqrt{2}} \quad \tau_6 = -\frac{1}{\sqrt{2}}$ all other coefficients 0

Solution 3: $\nu_2 = 1 \quad \nu_4 = -1 \quad \nu_5 = -\frac{1}{\sqrt{2}} \quad \nu_6 = \frac{1}{\sqrt{2}}$ all other coefficients 0

Solution 4: $\tau_2 = 1 \quad \nu_3 = -1 \quad \nu_5 = -\frac{1}{\sqrt{2}} \quad \nu_6 = -\frac{1}{\sqrt{2}}$ all other coefficients 0.

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 12. *G_W is an e_1-gate graph. A basis for the eigenspace of $A(G_W)$ with eigenvalue e_1 is*

$$|\chi_{1,a}\rangle = \frac{1}{\sqrt{3}}|\psi^1_{0,a}\rangle - \frac{1}{\sqrt{3}}|\psi^3_{0,a}\rangle - \frac{1}{\sqrt{6}}|\psi^5_{0,a}\rangle - \frac{1}{\sqrt{6}}|\psi^6_{0,a}\rangle \tag{6.25}$$

$$|\chi_{2,a}\rangle = \frac{1}{\sqrt{3}}|\psi^1_{1,a}\rangle - \frac{1}{\sqrt{3}}|\psi^4_{0,a}\rangle + \frac{1}{\sqrt{6}}|\psi^5_{0,a}\rangle - \frac{1}{\sqrt{6}}|\psi^6_{0,a}\rangle \tag{6.26}$$

$$|\chi_{3,a}\rangle = \frac{1}{\sqrt{3}}|\psi^2_{1,a}\rangle - \frac{1}{\sqrt{3}}|\psi^4_{1,a}\rangle - \frac{1}{\sqrt{6}}|\psi^5_{1,a}\rangle + \frac{1}{\sqrt{6}}|\psi^6_{1,a}\rangle \tag{6.27}$$

$$|\chi_{4,a}\rangle = \frac{1}{\sqrt{3}}|\psi^2_{0,a}\rangle - \frac{1}{\sqrt{3}}|\psi^3_{1,a}\rangle - \frac{1}{\sqrt{6}}|\psi^5_{1,a}\rangle - \frac{1}{\sqrt{6}}|\psi^6_{1,a}\rangle \tag{6.28}$$

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 (6.25) (and perhaps referring back to equation (6.5)) 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 11 we can write

$$|\Phi\rangle = \sum_{a,b\in\{0,1\},\, I,J\in[4]} C_{(I,a),(J,b)}|\chi_{I,a}\rangle|\chi_{J,b}\rangle \tag{6.29}$$

where the coefficients are symmetric, i.e.,

$$C_{(I,a),(J,b)} = C_{(J,b),(I,a)}, \tag{6.30}$$

and where

$$\langle\psi^q_{z,a}|\langle\psi^q_{x,b}|\Phi\rangle = 0 \tag{6.31}$$

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 (6.29)–(6.31) and prove the following.

Lemma 13. *A basis for the nullspace of $H(G_W, 2)$ is*

$$|\Phi_{a,b}\rangle = \mathrm{Sym}\left(\frac{1}{\sqrt{2}}|\chi_{1,a}\rangle|\chi_{3,b}\rangle + \frac{1}{\sqrt{2}}|\chi_{2,a}\rangle|\chi_{4,b}\rangle\right), \quad a, b \in \{0, 1\}. \tag{6.32}$$

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 (6.29) and (6.30), and one can directly verify that they also satisfy (6.31) (the nontrivial cases to check are $q = 5$ and $q = 6$).

To complete the proof that (6.32) 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 (6.31) gives

$$\langle\psi^1_{0,a}|\langle\psi^1_{0,b}|\Phi\rangle = \frac{1}{3}C_{(1,a),(1,b)} = 0 \qquad \langle\psi^1_{1,a}|\langle\psi^1_{1,b}|\Phi\rangle = \frac{1}{3}C_{(2,a),(2,b)} = 0$$
$$\langle\psi^2_{1,a}|\langle\psi^2_{1,b}|\Phi\rangle = \frac{1}{3}C_{(3,a),(3,b)} = 0 \qquad \langle\psi^2_{0,a}|\langle\psi^2_{0,b}|\Phi\rangle = \frac{1}{3}C_{(4,a),(4,b)} = 0$$
$$\langle\psi^1_{0,a}|\langle\psi^1_{1,b}|\Phi\rangle = \frac{1}{3}C_{(1,a),(2,b)} = 0 \qquad \langle\psi^2_{0,a}|\langle\psi^2_{1,b}|\Phi\rangle = \frac{1}{3}C_{(4,a),(3,b)} = 0$$
$$\langle\psi^3_{0,a}|\langle\psi^3_{1,b}|\Phi\rangle = \frac{1}{3}C_{(1,a),(4,b)} = 0 \qquad \langle\psi^4_{0,a}|\langle\psi^4_{1,b}|\Phi\rangle = \frac{1}{3}C_{(2,a),(3,b)} = 0$$

for all $a, b \in \{0, 1\}$. Using the fact that all of these coefficients are zero, and using equation (6.30), 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 (6.31) 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 11), 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

$$(i, j) \notin \{(1, 3), (3, 1), (2, 4), (4, 2)\} \quad\Longrightarrow\quad D_{(i,a),(j,b),(k,c)} = 0 \tag{6.33}$$

(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

$$(j, k) \notin \{(1, 3), (3, 1), (2, 4), (4, 2)\} \quad\Longrightarrow\quad D_{(i,a),(j,b),(k,c)} = 0 \tag{6.34}$$

$$(i, k) \notin \{(1, 3), (3, 1), (2, 4), (4, 2)\} \quad\Longrightarrow\quad D_{(i,a),(j,b),(k,c)} = 0. \tag{6.35}$$

Putting together equations (6.33), (6.34), and (6.35), we see that $|\Gamma\rangle = 0$. This is a contradiction, so no three-particle frustration-free states exist. □

Next we show how this gadget can be used to build gadgets the implement two-qubit gates.

6.2.2.1 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 (6.25)–(6.28). For each of the move-together gadgets $xy \in \{00, 01, 10, 11\}$ in Figure **??**, write

$$|\chi_{L,a}^{xy}\rangle$$

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 14. *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*

$$|\rho_{z,a}^{1,U}\rangle = \frac{1}{\sqrt{8}}|\psi_{z,a}^{1}\rangle - \frac{1}{\sqrt{8}}|\psi_{z,a}^{5+z}\rangle - \sqrt{\frac{3}{8}}\sum_{x,y=0}^{1}\tilde{U}(a)_{yz}|\chi_{1,a}^{yx}\rangle \quad |\rho_{z,a}^{2,U}\rangle = \frac{1}{\sqrt{8}}|\psi_{z,a}^{2}\rangle - \frac{1}{\sqrt{8}}|\psi_{z,a}^{6-z}\rangle - \sqrt{\frac{3}{8}}\sum_{x=0}^{1}|\chi_{2,a}^{zx}\rangle \tag{6.36}$$

$$|\rho_{z,a}^{3,U}\rangle = \frac{1}{\sqrt{8}}|\psi_{z,a}^{3}\rangle - \frac{1}{\sqrt{8}}|\psi_{z,a}^{7}\rangle - \sqrt{\frac{3}{8}}\sum_{x=0}^{1}|\chi_{3,a}^{xz}\rangle \qquad |\rho_{z,a}^{4,U}\rangle = \frac{1}{\sqrt{8}}|\psi_{z,a}^{4}\rangle - \frac{1}{\sqrt{8}}|\psi_{z,a}^{8}\rangle - \sqrt{\frac{3}{8}}\sum_{x=0}^{1}|\chi_{4,a}^{x(z\oplus x)}\rangle \tag{6.37}$$

where $z, a \in \{0, 1\}$. A basis for the nullspace of $H(G_U, 2)$ is

$$\mathrm{Sym}(|T_{z_1,a,z_2,b}^{U}\rangle), \quad z_1, z_2, a, b \in \{0, 1\} \tag{6.38}$$

where

$$|T^U_{z_1,a,z_2,b}\rangle = \frac{1}{\sqrt{2}}|\rho^{1,U}_{z_1,a}\rangle|\rho^{3,U}_{z_2,b}\rangle + \frac{1}{\sqrt{2}}\sum_{x_1,x_2=0}^{1} U(a)_{x_1x_2,z_1z_2}|\rho^{2,U}_{x_1,a}\rangle|\rho^{4,U}_{x_2,b}\rangle \tag{6.39}$$

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.

6.2.2.2 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 14 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 (6.36)–(6.37) and the other factor comes from the normalization in equation (6.5)), 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 (6.38) 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 15. *The smallest eigenvalue of $A(G_{bnd})$ is e_1, with corresponding eigenvectors*

$$|\rho^{bnd}_{z,a}\rangle = \frac{1}{\sqrt{8}}|\psi^{4}_{z,a}\rangle - \frac{1}{\sqrt{8}}|\psi^{8}_{z,a}\rangle - \sqrt{\frac{3}{8}}\sum_{x=0,1}|\chi^{x(z\oplus x)}_{4,a}\rangle. \tag{6.40}$$

There are no frustration-free states with two or more particles, i.e., $\lambda^1_N(G_{bnd}) > 0$ for $N \geq 2$.

6.2.3 Gate graph for a given circuit

6.2.3.1 Occupancy constraints graph

6.3 Proof of QMA-hardness for MPQW ground energy

6.3.1 Overview

6.3.2 Configurations

6.3.2.1 Legal configurations

6.3.3 The occupancy constraints lemma

6.3.4 Completeness and Soundness

6.4 Open questions

Chapter 7

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,

$$H_G^N\big|_{\mathcal{W}_N(G)} = O_G\big|_{\mathrm{Wt}_N(G)} \tag{7.1}$$

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 (7.1), i.e., the ground energy of O_G in the sector with magnetization N. We show that approximating this quantity is QMA-complete.

Problem 1 (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.

7.1 Relation between spins and particles

7.1.1 The transform

7.2 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

$$\lambda_N^1(G) = \min_{\substack{|\phi\rangle \in \mathcal{Z}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi|H_G^N - N\mu(G)|\phi\rangle \tag{7.2}$$

$$\leq \min_{\substack{|\phi\rangle \in \mathcal{W}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi|H_G^N - N\mu(G)|\phi\rangle \tag{7.3}$$

$$= \min_{\substack{|\phi\rangle \in \mathrm{Wt}_N(G) \\ \langle\phi|\phi\rangle = 1}} \langle\phi|O_G - N\mu(G)|\phi\rangle \tag{7.4}$$

$$= \theta_N(G) - N\mu(G) \tag{7.5}$$

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 (7.2)–(7.5)) that $\theta_N(G) - N\mu(G) > 0$, so

$$\theta_N(G) - N\mu(G) = \gamma\left(\left.(O_G - N\mu(G))\right|_{\mathrm{Wt}_N(G)}\right).$$

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

$$\begin{aligned}\gamma(H_B|_S) &= \gamma\left(\sum_{w=1}^{N}(A(G)-\mu(G))^{(w)}\big|_{\mathcal{W}_N(G)}\right)\\ &= \gamma\left(\left.(O_G - N\mu(G))\right|_{\mathrm{Wt}_N(G)}\right)\\ &= \theta_N(G) - N\mu(G).\end{aligned}$$

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. □

Chapter 8

Conclusions

There will definitely need to be some addition things here.

8.1 Open Problems

Heisenberg Modeaoeu

More simple graphs.

Is the constant term actually necessary?

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