The computational power of many-bodied systems

by

Zak Webb

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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.

Table of Contents

List of Figures

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.

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

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

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. This is probably the most analogous case to scattering off of a finite potential as in the 1-d continuum.

Because of this special form of the overall graph G, we know that the scattering eigenstates must take the

Note that even these simple models have a lot of computing power

I should really explain these NAND trees.

2.2.2 General graphs

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

$$A(\widehat{G}) = \begin{pmatrix} A & B^\dagger \\ B & D \end{pmatrix}, \tag{2.5}$$

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 $x \geq 2$ is an integer and $i \in [N]$, then the adjacency matrix for G will be

$$A(G) = A(\widehat{G}) + \sum_{j=1}^{N} \sum_{x=1}^{\infty} \big(|x, j\rangle\langle x+1, j| + |x+1, j\rangle\langle x, j| \big). \tag{2.6}$$

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

$$E = e^{ik} + e^{-ik} \tag{2.7}$$

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

$$\langle x, q \,|\, \mathrm{sc}_j(k) \rangle = \delta_{j,q} e^{ikx} + S_{qj} e^{ikx}. \tag{2.8}$$

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 Orthonormality of the scattering states

[**TO DO:** *Show that the scattering states are Delta function orthonormal*]

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

2.2.4 Scattering matrix properties

[**TO DO:** *I need to show that the scattering matrix is a unitary, and symmetric.*]

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

2.4.2 Momentum switches

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.

2.5.2 Not all momenta can be split

My interesting result.

Chapter 3

Universality of single-particle scattering

3.1 Finite truncation

I think I should include theorem 1 here (maybe)

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

Hard, but worthwhile

4.1 Multi-particle quantum walk

Note that this is exactly what I wanted to talk about.

Very difficult in general.

4.1.1 Two-particle scattering on an infinite path

The one thing we can actually compute It might be interesting to talk about what happens with spins.

4.2 Applying an encoded $C\theta$-gate

4.2.1 Finite truncation

Theorem 2

4.2.2 Construction of $C\theta$-gate

4.3 Impossibility of some momentum switches

4.4 Universal Computation

4.4.1 Two-qubit blocks

4.4.2 Combining blocks

4.5 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

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

This is a neat result for CS people.

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

6.2.1.1 The graph g_0

6.2.1.2 Gate graphs

Note that this will be different from our BH-paper, as I will include the doubling and self-loops

6.2.1.3 Frustration-free states for a given interaction range

6.2.2 Gadgets

6.2.2.1 The move-together gadget

6.2.2.2 Two-qubit gate gadget

6.2.2.3 Boundary gadget

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

7.1 Relation between spins and particles

7.1.1 The transform

7.2 Hardness reduction from frustration-free BH model

Chapter 8

Conclusions

8.1 Open Problems

Heisenberg Modeaoeu

More simple graphs.

References

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