

The computational power of many-bodied 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, one 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 P and NP with BQP and 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/universality 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

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

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

$$\langle x+1|\psi\rangle + \langle x-1|\psi\rangle = E_\psi \langle x|\psi\rangle. \quad (2.2)$$

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

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

If we then use the fact that E_ψ must be real, and that the amplitudes should not diverge to infinity as $x \rightarrow \pm\infty$, 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 known 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

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

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 G to an infinite path. This is probably the most analogous case to the s

2.2.1.1 R/T gadgets

One of the most simple cases of these scattering ideas is to simply attach a finite graph to a single vertex of an infinite path. Note that this is a restricted model of the above case, where $1 + A(k) = B(k)$ for all k .

2.2.1.2 General graphs

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

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

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 \hat{G} and N semi-infinite paths, with an additional edge between each of the first N vertices of \hat{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 $i \in [N]$,

Talk about scattering algorithms and AND trees.

2.2.2 Momentum switches

2.2.3 Applying an encoded unitary

2.3 Degree-3 graphs are sufficient

2.4 Multi-particle quantum walk

2.5 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.

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 Applying an encoded $C\theta$ -gate

4.1.1 Finite truncation

Theorem 2

4.1.2 Construction of $C\theta$ -gate

4.2 Impossibility of some momentum switches

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

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 Model

More simple graphs.

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