



NOTIONS OF ANALOGUE QUANTUM SIMULATION

Master's Project

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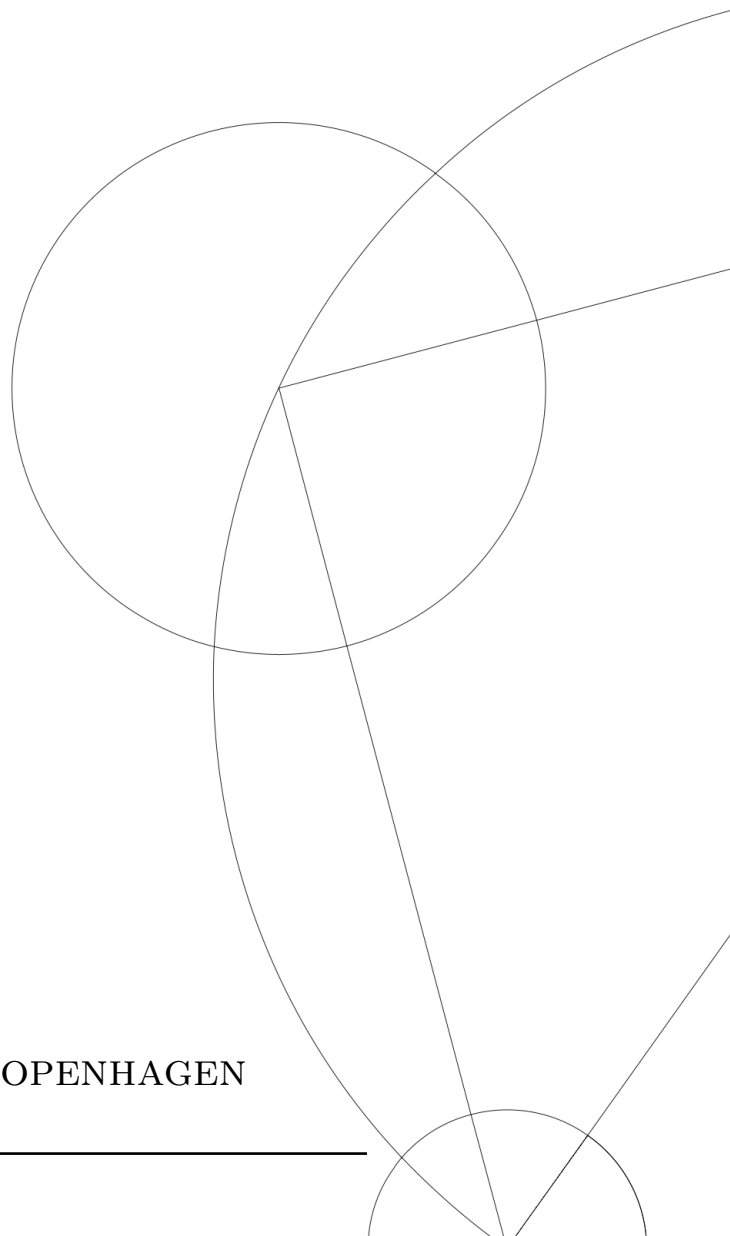
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Abstract

This master thesis explores the topic of analogue Hamiltonian simulation as a powerful method for simulating quantum systems. The thesis provides an introduction to the concept of analogue Hamiltonian simulation and its applications. It then discusses the concept of gadgets, which is used to construct more complex simulations. Perturbative gadgets from the literature are explored in detail, as are the author's own perturbative gadgets, such as the full geometric series and the direct k -local gadget. Logical gadgets, including the logical-AND from the literature and the novel chain gadget and logical swap, are also discussed, along with the introduction of the novel Magnus gadget heuristic. The work continues with a discussion of several relevant topics, such as simulations of Toffoli-gates under different connectivities, attempts to force a simulator Hamiltonian down into its low-energy-subspace, and a pro-con-like distinction between the Perturbative, Logical and Magnus gadgets. The thesis concludes with an application of all of these methods on the QuEra quantum-machine available from the AWS Braket program. Overall, the thesis provides a comprehensive overview to notions of analogue Hamiltonian simulation and their various applications.

Contents

1	Introduction	1
2	Analogue Hamiltonian Simulation	2
2.1	Notions of simulations	5
2.2	Notation and abuse of same	8
3	Universality	10
3.1	Logical Universality	10
3.2	Universal Gate Sets	10
3.3	Universal Simulators	12
4	Gadgets	14
4.1	Perturbative gadgets	14
4.1.1	Subdivision Gadget	18
4.1.2	3-to-2 Gadget	20
4.1.3	Full geometric series	22
4.1.4	Direct k-local Gadget	25
4.1.5	Simulations of error on Toffoli	29
4.1.6	Adding an error term	30
4.2	Logical Gadgets	32
4.2.1	Logical AND-gadget	33
4.2.2	Chain Gadget	34
4.2.3	Logical Swap	35
4.2.4	Combinations of Logical Gadgets	38
4.3	Magnus Gadgets	39
4.3.1	Magnus expansion	40
4.3.2	CNOT Construction	42
4.3.3	Toffoli Constructions	45
4.3.4	Numerical Simulations	47
5	Discussion	51
5.1	Toffoli Under Different Connectivities	51
5.2	Forcing qubits down into the low-energy-subspace	52
5.2.1	Couple to bath	53
5.2.2	Annealing	55
5.2.3	Protocols for testing	57
5.3	Strenghts and Weaknesses of Gadgets	60

6	Application	63
6.1	Perturbative Gadget	64
6.2	Logical Gadget	68
6.3	Magnus Gadget	71
6.4	Improved QuEra: Local on-site interactions.	73
6.4.1	Perturbative gadget: What if?	73
6.4.2	Logical gadget: What if?	75
6.4.3	Magnus Gadget: What if?	76
6.4.4	Cubitt-universality: What if?	77
7	Conclusion	79
8	Acknowledgements	80

1 Introduction

The development of quantum computers has sparked significant interest since physicist Paul Benioff's groundbreaking paper in 1980, where he proposed the idea of constructing a Turing Machine using a quantum model [3]. This concept gained further attention when Benioff and Richard Feynman discussed it at the First Conference on the Physics of Computation held at MIT in 1981, often considered as the birthplace of quantum computing [15]. Benioff presented his proof that every Turing machine can be stroboscopically simulated by a Hamiltonian's time-evolution, while Feynman emphasized the exponential infeasibility of classically simulating quantum systems as their size grows [12].

These early formulations are unified by their reliance on quantum analogue simulation, a distinct approach from the more commonly known digital quantum computers. Digital computers manipulate universal bits to perform logical operations, whereas analogue simulations operate closer to the underlying hardware. Specifically, analogue simulations aim to simulate one model with another model, focusing on the approximation of Hamiltonians rather than the manipulation of states through applied gates.

In this master's thesis, we delve into the approximation of one Hamiltonian using another. Our objective is to approximate the interactions of Hamiltonians that couple numerous qubits through Hamiltonians acting on fewer qubits. We accomplish this within the framework of Hamiltonian gadgets, a technical tool available in the literature for mimicking one Hamiltonian with another. While one might assume that simulations involve minimizing the matrix-norm difference between the two Hamiltonians, we explore different notions of simulation, each leading to distinct notions of universality in terms of simulatability and applicability in regards to the introduced gadgets of this thesis.

The thesis proceeds as follows: In Section 2, we provide a brief technical overview of our research objectives and motivation. In section 3 we discuss various notions of universality, encompassing logical universality, universal quantum gate sets, and universal simulatability. In Section 4, we introduce three distinct gadgets examined in this thesis: The Perturbative gadget (Section 4.1), the logical gadget (Section 4.2) and the novel Magnus gadget (Section 4.3). Section 5 delves into the underlying assumptions associated with these gadgets and highlights their points of divergence. Finally, in Section 6, we apply the three gadgets to the QuEra hardware, an ion-trap quantum computer that positions itself as an analogue quantum simulator.

By exploring the strengths, weaknesses, and applications of these gadgets, this thesis contributes to our understanding of Hamiltonian simulation and its potential within the emerging field of quantum computing.

2 Analogue Hamiltonian Simulation

In this thesis, we will consider problems of quantum systems on graphs with finite local dimension such as a system of interacting spins. Formally this means that we model a Hilbert space that locally consists of spaces $\mathcal{H}_i = \mathbb{C}^{d_i}$ for some finite d_i , set to 2 when working with qubits, and have the total Hilbert space $\mathcal{H} = \bigotimes_{i \in V} \mathcal{H}_i$ on the graph (V, E) . We do this because of its relevance to quantum computers that work on finite clusters of qubits with fixed connectivity graphs and because a typical first approximation of many condensed matter systems relevant to material physics are finite-state models on lattice-graphs.

In quantum mechanics, local operators play a crucial role in describing the physical properties and behavior of quantum systems. Local operators are operators that act non-trivially only on a small subset of the total system, typically on a single or few qubits, and do not affect the rest of the system. Formally, a k -local operator is defined to be an operator whose terms act on at most k vertices. Mathematically, denote by Per_π the operator that acts as the permutation π on the ordering of our qubits. Then an operator is k -local if for each of its terms there exists permutations π_n such that the Hamiltonian can be written:

$$H = \sum_{n=1}^N H_n, \quad \text{Per}_{\pi_n} H_n \text{Per}_{\pi_n}^{-1} = \widetilde{H}_n \otimes \mathbb{1}_{\text{rest},n}$$

That is, up to permutation, each term acts non-trivially only by \widetilde{H}_n . In order to be k -local, we furthermore demand each such \widetilde{H}_n to act on at most k qubits. See figure 1 for a schematical representation of this definition. If the Hamiltonian in particular can be written in the simple form:

$$H = \bigotimes_{i=1}^K A_i$$

We will refer to H as a product operator. The locality of such an operator is the amount of factors A_i 's which are non-trivial.

Notice that by this convention, an operator of "high locality" means a k -local operator with large k and thus one that makes many qubits interact. Conversely, an operator of "low locality" makes few qubits interact. This might seem counter-intuitive in the sense that one could refer to an operator as "highly" local to establish that it didn't couple qubits far apart, but we will in this thesis consistently denote "high" or "low" locality to refer to whether the number k of a k -local operator is high or low.

The locality of these operators reflects the idea that physical interactions between particles are typically local, meaning that they only couple a few particles at the same time. In nature, most physical interactions observed are characterized as two-particle interactions. 3-particle scattering

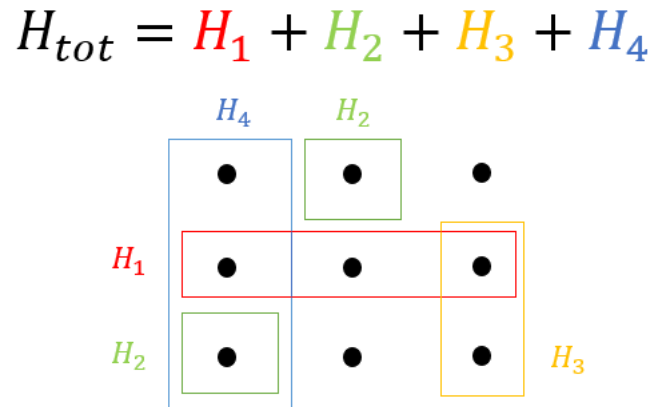


Figure 1: Schematical drawing of a 3-local Hamiltonian. Notice that not all interactions have to act on 3 qubits and that the qubits that are coupled don't have to be geometrically close.

events do exist but are much more difficult to have total control over in a lab and thus we will think of them as rare or difficult to implement.

We have established which systems we will model and how we will distinguish them by the locality of their interaction. We will now go on to say how we model their dynamics from their Hamiltonian.

The dynamics of any closed quantum system is governed by the Schrödinger equation [14]. For time-independent problems it takes the well-known form in natural units $\hbar = 1$:

$$i\hbar \frac{d\psi}{dt} = H\psi(t)$$

The solution to this problem can be represented through the time-evolution operator $U(t)$ that models the dynamics of states:

$$\psi(t) = U(t)\psi(0)$$

For the time independent problem the time-evolution operator $U(t) = \exp(-itH)$ forms a strongly-continuous, one-parameter unitary group meaning that:

$$U(t)^\dagger = U(t)^{-1} = U(-t), \quad U(t+s) = U(t)U(s)$$

For which the Hamiltonian acts as the generator. We are able to recover this interaction from the time-evolution by:

$$-iH(t) = \lim_{\Delta t \rightarrow 0} \frac{U(t + \Delta t) - U(t)}{\Delta t} \equiv \frac{d}{dt}U(t)$$

Where the limit should be understood as taken w.r.t, the operator norm defined as:

$$\|A\| \equiv \sup_{\psi \in \mathcal{H} \setminus \{0\}} \frac{\|A\psi\|}{\|\psi\|}$$

Which is a definition of operator norms we will consistently use throughout this thesis. Thus, we can always go from the interactions of a quantum system to its dynamics via the time-evolution operator, or from its dynamics to an interaction through the derivative.

As hinted at above, Hamiltonians of large locality can become very complex in regards to implementability and predicatability as physical models. Implementing a Hamiltonian typically involves the manipulation of the physical system, such as the application of magnetic or electric fields. However, implementing a Hamiltonian of large locality experimentally requires a significant amount of resources, making it difficult or even impossible in some cases. This leads the way for the concept of analogue Hamiltonian simulation: The idea that one Hamiltonian might be able to simulate or approximate the dynamics of another. By approximating a Hamiltonian of high locality (referred to as a “target Hamiltonian”) with a Hamiltonian of low locality (referred to as a “simulator Hamiltonian”), it becomes easier to experimentally implement the target Hamiltonian. Should such a simulator Hamiltonian exist, it might allow for the study of complex systems and phenomena in a smaller, more manipulable environment that would otherwise be challenging to investigate.

Such a mapping between high locality target Hamiltonians and low locality simulator Hamiltonians is not always straightforward, as the simpler Hamiltonian may not have enough free parameters to fully capture the complexity of the original Hamiltonian. To address this, an ancilla qubit is often introduced to the system. By doing so, more free parameters can be adjusted in the simulator Hamiltonian, ideally allowing for a better approximation of the target Hamiltonian. However, introducing an ancilla qubit also means that the Hilbert space of the system becomes larger than that of the original Hamiltonian. Thus, when viewed operationally, the simulator Hamiltonian can’t have the same action as the target Hamiltonian in the sense that the two operators can’t be compared naturally. To address this, the simulator Hamiltonian will be restricted to a subspace of the Hilbert space, typically the low-energy subspace. The main experimental justification hereof is foremost that any closed quantum system will conserve its expected energy under the influence of a time-independent interaction and thus will stay in a low-energy-state given that it started there. Secondary, a system of well-defined and low temperature will be approximately contained in its low-energy subspace, so it’s a meaningful approximation for many condensed matter systems.

The technical part of analogue Hamiltonian simulation will in this thesis be realized via a technique called Hamiltonian gadgets or just gadgets for short. They were originally introduced as an

attempt to solve the " k -local-Hamiltonian problem"; a promise problem that consists of figuring out whether a k -local Hamiltonian has a ground state energy above or below some given threshold. The Perturbative gadget was introduced in [18] to prove that the ground-state energy of any k -local Hamiltonian with $k \geq 2$ can be simulated via Hamiltonians that are 2-local and in this regard they proved universal simulability of the 2-local-Hamiltonian problem. By the knowledge that the " k -local-Hamiltonian problem" is QMA-complete, they proved QMA-completeness of the "2-local-Hamiltonian Problem" and also universal simulatability of 2-local Hamiltonians in the context of the complexity class QMA. But this means that Gadgets were originally introduced as a means to approximate the lowest energy of a given Hamiltonian. Because much work has been done since to generalize their use, gadgets can now simulate the dynamics of a Hamiltonian of higher locality as well as simulate its eigenvalues. This inspires us to discuss various notions of simulation in the next section.

2.1 Notions of simulations

In this section, we will define and discuss different notions of Hamiltonian simulation. One can convey many different things when saying that one Hamiltonian simulates another. There are three naïve versions, which we'll introduce now from weakest to strongest concept.

The first version is the approximate simulation of the low-energy spectrum of a given Hamiltonian. This means that for fixed Δ the simulator Hamiltonian have eigenvalues $\lambda_{\text{sim},i} \leq \Delta$ that are close to the eigenvalues of the target Hamiltonian $\lambda_{\text{target},i}$:

$$\max_i |\lambda_{\text{sim},i} - \lambda_{\text{target},i}| \leq \varepsilon$$

For some $\varepsilon > 0$ and for all eigenvalues below the fixed energy threshold Δ . In this approach, the low-energy section of the simulator is designed to capture the most essential feature of the system, namely its energies which is often the most important aspect for practical applications. However, no relation to the eigenstates are assumed, which governs the dynamics of the system.

A second version of Hamiltonian simulation concerns the approximate simulation of the time-evolution of a Hamiltonian as an operator. That is:

$$\|U_{\text{sim}}(t) - U_{\text{target}}(t)\| \leq \varepsilon$$

For some $\varepsilon > 0$. This bound can either be uniform in time or be indexed by time and work stroboscopically.

This approach involves constructing a simulator that can evolve a given state forward in time under the Hamiltonian, providing approximate insights into the dynamics of the system. We will

in this work only concern ourselves with the time-evolution operator at single points in time and thus not use uniform bounds of ε .

The third version is the most naïve one but also the strongest: Constructing an approximate simulation of the full Hamiltonian viewed as an operator.:

$$\|H_{\text{sim}} - H_{\text{target}}\| \leq \varepsilon$$

In this approach, the simulator is designed to mimic the full dynamics of the Hamiltonian. This is what we'll set out to do most of the time in this thesis, and we will specify whenever we attempt any other sort of simulation.

It is obvious that the simulation of the full Hamiltonian implies the simulation of its eigenvalues but that the simulation of the full Hamiltonian implies simulation of the time-evolution can be shown as a small application of the fundamental theorem of calculus. Define $\Delta H = H_{\text{target}} - H_{\text{sim}}$ and assume that $\|\Delta H\| \leq \varepsilon$. Then, for any time-independent problem, we have by the triangle inequality:

$$\begin{aligned} \|U_{\text{target}}(t) - U_{\text{sim}}(t)\| &= \|\exp(-itH_{\text{target}}) - \exp(-itH_{\text{sim}})\| = \|\exp(-it\Delta H) - \mathbb{1}\| \\ &= \left\| \int_0^t \frac{d}{ds} \exp(-is\Delta H) ds \right\| = \left\| \int_0^t -i\Delta H \exp(-is\Delta H) ds \right\| \leq \int_0^t \|\Delta H\| ds \leq t\varepsilon \end{aligned}$$

And thus, simulability of an interaction to error ε implies simulability of the time-evolution with at most error $t\varepsilon$.

The intuition behind the three ideas of simulability above are clear in an operational sense, whilst it is also clear that their goals are very different. Simulating eigenvalues is perfect for answering the " k -local-Hamiltonian problem". Approximating the time-evolution makes sense when one is only curious about the state of a system after some process, like in the context of quantum computers. To simulate the whole Hamiltonian is needed if one attempts to actually simulate the interactions of a system, and thus the last notion of simulability can be used as a probe for imitating complex physical models.

There exists a fourth framework introduced by Toby Cubitt et al. [10] that works a bit differently than the three naïve notions, but which generalizes the above ideas and we'll introduce it in the following section. In [10] they refine the idea of being able to compare two Hamiltonians via the concept of "Encodings". An encoder should be interpreted as a dictionary that maps a target Hamiltonian from the space it acts on onto the space that the simulator Hamiltonian acts on such that the two can actually be compared in the same language. A mapping $\mathcal{E} : B(\mathcal{H}) \rightarrow B(\mathcal{H}')$ is

called an encoding if the following three conditions are upheld:

$$\mathcal{E}(A) = \mathcal{E}(A)^\dagger, \text{ if } A = A^\dagger. \quad (1)$$

$$\text{Spec}(\mathcal{E}(A)) = \text{Spec}(A) \quad (2)$$

$$\mathcal{E}(aA + bB) = a\mathcal{E}(A) + b\mathcal{E}(B) \text{ for any real } a \in [0, 1], b = 1 - a \text{ and hermitian } A, B \in B(\mathcal{H}). \quad (3)$$

These criteria are physically motivated: The first implies that an encoder sends hermitian operators to hermitian operators, which means that it maps physically feasible Hamiltonians to other physically feasible Hamiltonians. The second criteria states that the operator and encoding have the same energies and the third states that sums of different parts of your Hamiltonian gets sent to sums of different parts of the encoding. The last is a sufficient condition to get that classical probabilistic mixtures of two observables get the same expectation value in the encoder and in the simulator for all states. [10]

These three conditions have been proven by Cubitt et al. to imply that many more physical properties of the Hamiltonian are reproduced by the encoder such as conservation of the partition function and that the encoder has many other mathematical properties like real-linearity. They furthermore prove that these three criteria imply a characterization of all encoders to be of the form:

$$\mathcal{E}(H) = U(H^{\oplus p} \oplus \overline{H}^{\oplus q})U^\dagger$$

for some unitary U , non-negative integers p and q and where $\overline{}$ denotes complex conjugation of each entry in H . The characterization can equivalently be written as:

$$\mathcal{E}(H) = U(H \otimes P + \overline{H} \otimes Q)U^\dagger$$

For some orthogonal projectors P and Q that have $P + Q = \mathbb{1}$.

If the encoding only has support on a subspace $S \subseteq \mathcal{H}'$ of the target space, a comparison between simulators and encodings can still be made and thus, it makes sense to characterize such encoders. There, the characterization instead becomes:

$$\mathcal{E}(H) = V(H \otimes P + \overline{H} \otimes Q)V^\dagger$$

For some isometry $V : S \rightarrow \mathcal{H}$. Typically, we will distinguish between local and non-local encodings by whether or not V can be written as a product-operator $V = \bigotimes_j V_j$.

With the ground work set, Cubitt et al. proceed to define a Hamiltonian simulation to be when an encoding of a target Hamiltonian becomes equal to a simulator Hamiltonian constricted to some subspace of the larger Hilbert space. In practise, the subspace they're referring to is always the low-energy subspace of the simulator Hamiltonian. In mathematical terms, in order for one

Hamiltonian to simulate another, there has to exist an encoding \mathcal{E} and an energy-cutoff Δ such that:

$$\begin{aligned}\mathcal{E}(\mathbb{1}) &= P_{\leq\Delta} \\ H_{\text{sim}}P_{\leq\Delta} &= \mathcal{E}(H_{\text{target}})\end{aligned}$$

Where $P_{\leq\Delta}$ denotes the projection onto the low-energy-subspace of H_{sim} . This warrants a natural way to think of exact simulations but there is a need to discuss approximate simulations, since these typically aren't without errors. We say that a simulator Hamiltonian simulates a target Hamiltonian to precisions $\eta, \varepsilon > 0$ below energy threshold Δ when there exists a (not necessarily local) encoding

$$\tilde{\mathcal{E}}(H_{\text{sim}}) = \tilde{V}(P \otimes H_{\text{sim}} + Q \otimes \overline{H_{\text{sim}}})\tilde{V}^\dagger$$

such that the two following conditions are upheld:

$$\begin{aligned}\|V - \tilde{V}\| &\leq \eta \\ \|H_{\text{Target}}P_{\leq\Delta} - \tilde{\mathcal{E}}(H)\| &\leq \varepsilon\end{aligned}$$

In this way Cubitt et al. have introduced a full concept of Hamiltonian simulation, both exact and approximate. We will refer to this framework as Cubitt-simulation and come back to this version of simulation in section 6 whilst analyzing the QuEra quantum computer.

In the next section, we will rapidly go over the notation we will use in this thesis.

2.2 Notation and abuse of same

We will use conventions from the literature of quantum theory. We assume knowledge of the notion of the Pauli matrices and the ‘‘number operator’’:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad N^\sigma = \frac{1}{2}(\mathbb{1} - \sigma), \quad \overline{N}^\sigma = \mathbb{1} - N^\sigma$$

For $\sigma \in \{X, Y, Z\}$. Notice that the counting operator N^σ is a projection onto the eigenstate of σ which has eigenvalue -1 and the ‘‘non-counting operator’’ \overline{N}^σ is a projection onto the eigenvalue 1 .

During this thesis, we will abuse notation in how we will denote tensor products in the following sense: Assume we have N qubits on the Hilbert Space $(\mathbb{C}^2)^{\otimes N}$. We denote the operator that only acts on qubit k by:

$$A_k \text{ ‘‘=’’ } \bigotimes_{i=1}^{k-1} \mathbb{1} \otimes A_k \otimes \bigotimes_{i=k+1}^N \mathbb{1}$$

from this notation, products of operators acting on different spaces act exactly like tensor products. That is for $n \neq m$:

$$A_n A_m \text{ “ = ” } \left(\bigotimes_{i=1}^{n-1} \mathbb{1} \otimes A_n \otimes \bigotimes_{i=n+1}^N \mathbb{1} \right) \left(\bigotimes_{i=1}^{m-1} \mathbb{1} \otimes A_m \otimes \bigotimes_{i=m+1}^N \mathbb{1} \right) \text{ “ = ” } A_n \otimes A_m$$

So by this abuse of notation, tensor products aren't always explicitly stated. Instead, it should be clear from context which space the operators act on and in what sense they should be multiplied. In the next section, we will introduce three different notions of universality. This will be useful in section 4 and onward when utilizing these concepts.

	NAND(\cdot)	NOR(\cdot)
00	1	1
01	1	0
10	1	0
11	0	0

Table 1: Truth table for the two universal logical clauses NAND and NOR.

3 Universality

We will in this thesis use the word "universality" in a variety of different contexts. Therefore, it makes sense to point out in which contexts we will utilize it and what we mean by it such that our terminology stands clear before we introduce the technical work. We will swiftly introduce the concept of "logical universality" in the context of logical statements, discuss "universal gate sets" in the context of quantum gates and end with "universal simulators" in the context of the Cubitt-simulation notion.

3.1 Logical Universality

Formally, a logical statement is a mapping from some number of Boolean variables to a single Boolean variable, which we will call a literal. We typically represent logical statements with truth tables, which are lists of what outputs one gets from the mapping for all inputs.

Any finite logical statement can be decomposed into compositions of finitely many smaller logical statements on literals. If we have a set of statements that under compositions can replicate any truth table, we call such a set a universal logic set and will refer to this property as "logical universality" during the thesis. There exists strong results on which logical statements are universal; two examples of these are the universal NAND- and the universal NOR operations [23] respectively defined by truth table in table 1. We will solely refer to the universality of either of these two operations in the technical work onward, especially in section 4.2 that concerns the Logical gadget.

3.2 Universal Gate Sets

Digital quantum computers canonically work via the application of unitary gates of high fidelity onto well-controlled quantum states such that a measurement of the state will hold information about a problem that is sought to be solved. The strongest version of such a quantum computer should be able to apply any possible unitary operator at least approximately in a feasible manner with respect to the resources it holds native. Inspired hereof, there exists the concept of a "universal gate set". Such a gate set S is defined to be able to apply any unitary on n qubits

$U : \mathbb{C}^{2^n} \rightarrow \mathbb{C}^{2^n}$ up to error ε by applying t gates from S , where $t = \text{poly}(n, \frac{1}{\varepsilon})$ [1]. Universal gate sets include the rotation gate set with a CNOT: $\{R_x(\theta), R_y(\theta), R_z(\theta), \text{CNOT}|\theta \in \mathbb{R}\}$, the Clifford gate set with a T -gate, and the gate set consisting of only the Hadamard and Toffoli gates. This thesis places particular emphasis on the Toffoli gate set, as it only consists of two gates and it is unique in the sense that its only challenging aspect is producing a three-local unitary. This challenge is ideally suited for the framework of this thesis and therefore, it is worthwhile to delve deeper into the Toffoli gate's properties.

We denote the Toffoli gate in the standard basis:

$$\text{Toff} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} = C_1 C_2 X_3$$

It is also referred to as a controlled-controlled-not-gate; we flip the third bit if and only if the two first bits are 1. We can get it from the following 3-qubit interaction:

$$H_{\text{Toff}} = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix} = N_1^z \otimes N_2^z \otimes N_3^x$$

In the sense that:

$$\text{Toff} = \exp(-i\pi H_{\text{Toff}})$$

We will repeatedly get back to this operator as an example of a target Hamiltonian in the application of gadgets, and luckily it has the simple form of a product operator consisting of on-site interactions making it a prime candidate for locality simplifications.

By the universality of certain 2-qubit gates and all 1-qubit gates, it is clear that the Toffoli can instead be made as a successive application of CNOT's and 1-qubit gates. Our hope for this project is that our attempts at simulation does better at constructing this gate than any

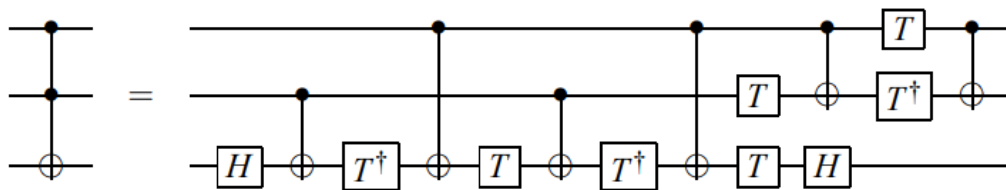


Figure 2: Decomposition of a Toffoli Gate into 2- and 1-qubit gates from [26]. The quantum circuit formalism is canonical in the literature and is read from left to right in order of application. A black dot means that the operation it is connected to is controlled on this bit and a plus is standard diagrammatic notation for a NOT gate. The construction requires 6 CNOT’s and 9 1-qubit gates. The optimality of 6 CNOTS has been proven in [26].

decomposition from CNOT’s and 1-qubit-gates in the context of either time resources or implementability complexity. A typical decomposition of the Toffoli looks like the circuit of figure 2. It consists of 6 CNOT’s and 9 on-site gates. The figure comes from the work [26] that also proves that the toffoli gate cannot be constructed more efficiently than by using 6 CNOT’s.

In general, this gate can easily reconstruct the effect of any other Control-control- U -gate, where U is a 1-qubit unitary operator, since they are equivalent up to applications of 1-local unitary operations.

3.3 Universal Simulators

In regards to analogue Hamiltonian simulations, one denotes universal simulability as the property of a class of Hamiltonians, typically parameterized by tunable parameters, to be able to simulate any Hamiltonian. Originally, [18] used the perturbative gadget to prove universality of 2-local Hamiltonians in regards to the k -local-Hamiltonian problem. That is of course a sort of simulation universality, but we are equally interested in simulating the dynamics of a Hamiltonian as we are curious about its energies. Here we for instance know that the universal gate sets (or the Hamiltonians that generate these gates) form universal simulators in the sense of simulating time-evolutions.

Cubitt et al. also made a classification of Hamiltonians that simulate all other Hamiltonians in the context of Cubitt-simulation. Concretely, they found 2-local Hamiltonians with no Pauli-Y-component in their Pauli decomposition to be able to simulate any interaction, that is models of the form:

$$H = \sum_{i>j} \alpha_{ij} A_{ij} + \sum_k \beta_k X_k + \gamma_k Z_k \tag{4}$$

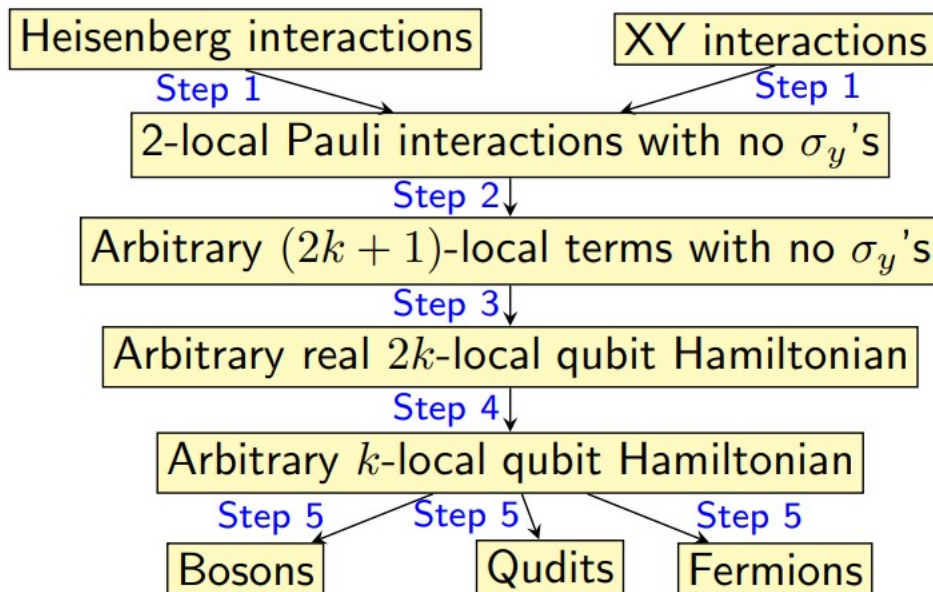


Figure 3: Simulatability of the Cubitt-framework from [10]. The figure shows which classes of Hamiltonians that can simulate others, where an arrow indicates that the class at the arrow tail can simulate the class at the arrow head. The steps in the figure refer to the order in which Cubitt et al. prove simulability of all Hamiltonians from the Heisenberg and XY-interactions. We will in this thesis just focus on the 2-local Pauli-interactions with no Y 's in section 6.4.4.

where $A_{ij} \in \{Z_i Z_j, X_i Z_j, Z_i X_j, X_i X_j\}$ and for general real $\alpha_{ij}, \beta_k, \gamma_k \in \mathbb{R}$.

This is in no way an exhaustive characterization: Cubitt et al. finds many classes of Hamiltonians that are universal in the sence of simulability in their framework. For details on which Hamiltonians are universal in the Cubitt-framework, we refer to figure 3 which comes from their own work on universal Hamiltonian simulators.

In the next section, we will commence our technical work on Hamiltonian gadgets. We will introduce the three gadgets of this thesis and apply them for many different construction.

4 Gadgets

Gadgets are the mathematical toolbox we will utilize for proving simulatability of Hamiltonians from less complex Hamiltonians in this thesis but they might also provide a practical protocol on how one can implement complex Hamiltonians using fewer computational resources. There are many kinds of gadgets and they have each their respective strengths and faults. In this section, we will present the Perturbative gadget construction by [18], the Logical gadget construction by [4] and construct a novel class of gadgets which we will call Magnus gadgets.

4.1 Perturbative gadgets

The first example of a Perturbative gadget was written in an appendix as an alternative way to prove the universality of 3-local Hamiltonians in the k -local Hamiltonian problem [18]. The framework was general enough to spark significant inspiration and ended up producing many simulation results in the literature that followed.

The framework uses methods well known in the literature of physics. We will utilize what condensed matter physicists call renormalization of the Green's function to approximate dynamics of a Hamiltonian after applying a perturbation. Notice that the words "resolvent", "Green's function" and "propagator" will be used interchangeably, as they mean the same thing but in three different scientific fields. To initiate the framework, we will start out by making a decomposition of our Hilbert Space into states contained in the low-energy-subspace and states contained in the high-energy-subspace of our Hamiltonian. That is for some real number $\lambda_* \in \mathbb{R}$, we make the distinction:

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$$

For which $\mathcal{H}_- = \text{span}\{|\psi\rangle \mid \langle\psi|H\psi\rangle \leq \lambda_*\}$ and $\mathcal{H}_+ = \text{span}\{|\psi\rangle \mid \langle\psi|H\psi\rangle > \lambda_*\}$. For an operator X on \mathcal{H} , we denote:

$$X_{++} = P_+XP_+, \quad X_{+-} = P_+XP_-, \quad X_{-+} = P_-XP_+, \quad X_{--} = P_-XP_-$$

Where P_{\pm} respectively denotes the projection onto \mathcal{H}_+ and \mathcal{H}_- . Heuristically, the method then starts out with the resolvent of a given Hamiltonian:

$$G(z) = \frac{1}{z\mathbb{1} - H}$$

The poles of G exactly corresponds to the eigenvalues of H [18]. After perturbing our Hamiltonian:

$$\tilde{H} = H + V$$

We get another Greens function that relates to the previous Green's function:

$$\tilde{G}(z) = \frac{1}{z\mathbb{1} - \tilde{H}} = (G^{-1} - V)^{-1}$$

We can write all these objects in block-form with respect to the subspaces of \mathcal{H}_- and \mathcal{H}_+ as:

$$H = \begin{pmatrix} H_{--} & 0 \\ 0 & H_{++} \end{pmatrix}, \quad V = \begin{pmatrix} V_{--} & V_{+-} \\ V_{-+} & V_{++} \end{pmatrix},$$

$$G = \begin{pmatrix} G_{--} & 0 \\ 0 & G_{++} \end{pmatrix}, \quad \tilde{G} = \begin{pmatrix} \tilde{G}_{--} & \tilde{G}_{+-} \\ \tilde{G}_{-+} & \tilde{G}_{++} \end{pmatrix}$$

And we define the “self-energy” to be:

$$\Sigma(z) = z\mathbb{1}_{--} - (\tilde{G}^{-1})_{--}$$

The intuition behind this definition is that this object would be the total Hamiltonian if we were completely confined to the low-energy subspace. But since the perturbation leaks states between high- and low-energy, we get that the self-energy both contains information about how the low-energy perturbed Hamiltonian looks but also how the off-diagonal entries of the perturbation $V_{\pm\mp}$ give transition amplitudes between the low- and high-energy subspaces of \mathcal{H} .

From the Schur-complement-formula on how to invert block-matrices [13], we get a formula for the self-energy:

$$\begin{aligned} \Sigma(z) = z\mathbb{1}_{--} - (\tilde{G}^{-1})_{--} &= H_{--} + V_{--} + V_{-+}((G^{-1})_{++} - V_{++})^{-1}V_{+-} \\ &= H_{--} + V_{--} + V_{-+}G_{++}(1 - G_{++}V_{++})^{-1}V_{+-} \end{aligned}$$

Up to this point, everything we have done has been analytical but the following step is where one can utilize perturbation theory. Given a criterion for convergence, one can expand the term in the middle as a Neumann series or a geometric series to get:

$$\Sigma(z) = H_{--} + V_{--} + \sum_{n=0}^{\infty} V_{-+}G_{++}(G_{++}V_{++})^nV_{+-}$$

In all applications of the perturbative gadget we have in this section, our unperturbed Hamiltonian H will be of the form:

$$H = \Delta N_m^z$$

Where N_m^z is the counting operator acting on some ancilla qubit m and Δ is a gap parameter we will think of as large. Notice that we will think of objects with the subscript m as ancilla qubits or operators acting on ancilla qubits throughout this thesis.

The high-energy-subspace is thus characterized by only an ancilla qubit being its high energy state with an energy gap of Δ . Therefore the non-perturbed high-energy propagator has the simple form:

$$G_{++}(z) = P_+ \frac{1}{z\mathbb{1} - H} P_+ = \frac{1}{z - \Delta} |1\rangle \langle 1|_m$$

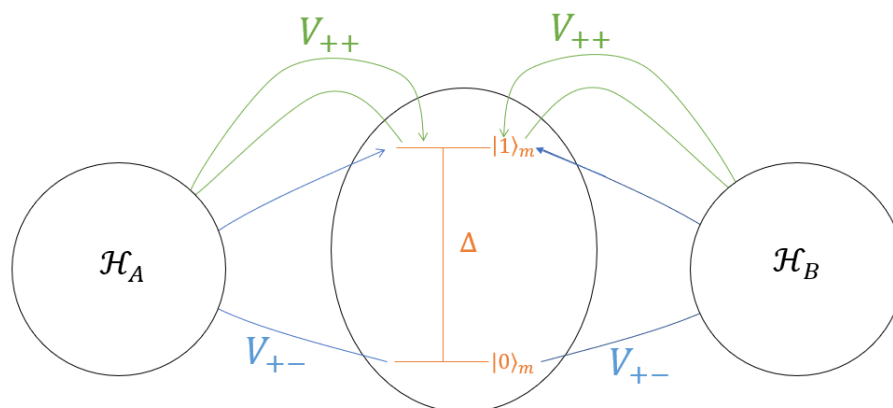


Figure 4: Schematic of how the Perturbative gadget works. By coupling the terms that excite or relax the ancilla qubit with systems \mathcal{H}_A and \mathcal{H}_B , we can simulate virtual interactions between \mathcal{H}_A and \mathcal{H}_B from the change in self-energy.

And thus, the above geometric series becomes:

$$\Sigma(z) = H_{--} + V_{--} + \sum_{n=0}^{\infty} \frac{V_{-+}(V_{++})^n V_{+-}}{(z - \Delta)^{n+1}} \quad (5)$$

If $\|\frac{V}{\Delta}\|$ is small, this can be seen as a perturbative expansion in V which can be truncated to finite order. The physical intuition is that the self-energy changes by the perturbation to induce virtual interactions between other systems than the ancilla qubit, see figure 4 for a schematical representation.

Now, Kempe et al. collected all of these heuristics by proving the following theorem:

Theorem 1. *Assume a simulator Hamiltonian of the form $H_{sim} = H_0 + V$ where the unperturbed Hamiltonian H_0 has spectral gap of size Δ around λ_* and that $\|V\| \leq \Delta/2$. For arbitrary $\varepsilon > 0$, if there exists an operator H_{target} with $\text{spec}(H_{target}) \subseteq [c, d]$ which $\forall z \in (c - \varepsilon, d + \varepsilon)$ has that:*

$$\|\Sigma(z) - H_{target}\| \leq \varepsilon$$

Then each eigenvalue λ_n of H_{target} is ε close to each eigenvalue of $(H_{sim})_{\leq \Delta}$

The strength of the method comes from perceiving the expansion of equation 5. One can truncate the geometric series as a recipe for simulating target Hamiltonians through H_{sim} within a certain error. To analyze this error, we will need to expand the Green's functions in their Laurent series in z to get the object to zeroth order such that we can apply Theorem 1. The art of the method

then comes from finding a good choice for H_{sim} .

The strength of the Perturbative gadget is that we can construct non-local interactions, since the terms in the expansion go like $(V_{++})^n$. The method is also very close to perturbative methods of quantum field theory and condensed matter theory and has thus been studied a lot, although rarely to such a mathematical extent where the error is bounded.

Notice that the gadget has two apparent weaknesses: First, it demands that we remain in the low-energy subspace of our Hilbert Space, that is, there is no promise for how well the simulation would go were we in the high-energy subspace. Second, even after making sure that we are confined to the low-energy subspace, it only simulates Hamiltonians within some error threshold. In this thesis, we will bound the asymptotic error as a function of the energy gap parameter. A relevant question one could ask is whether one can apply a strong enough gap Δ to get within the error threshold one would want in an actual experimental simulation, but we will not attempt to answer this question in the following work.

The framework introduced by [18] was a statement about the eigenvalues being simulatable. In the paper, the authors also proved that the construction of Theorem 1 implied that the ground state was simulated up to small error. Actually, the work they did worked for all energies and states of the low-energy-subspace without many further technicalities, so the mantle was taken up from there and the method was strengthened to be a norm bound instead of a bound on differences on eigenvalues in [24]:

Lemma 1. *Assume we're in the same scenario as in Theorem 1 and that $P_- H_{\text{target}} P_- = H_{\text{target}}$. Let D_r denote the circle with radius r in the complex plane with $w_+ = \frac{d+c}{2}$ as center. Let r be such that $d + \varepsilon < w_+ + r < \lambda_*$, and let $w_- = \frac{d-c}{2}$. Assume that $\forall z \in D_r$ we have:*

$$\|\Sigma(z) - H_{\text{target}}\| \leq \varepsilon$$

Then:

$$\|(H_{\text{sim}})_{\leq \Delta} - H_{\text{target}}\| \leq \frac{3(\|H_{\text{target}} + \varepsilon\|)\|V\|}{\lambda_+ - \|H_{\text{target}}\| - \varepsilon} + \frac{r(r + w_-)\varepsilon}{(r - w_+)(r - w_+ - \varepsilon)} \equiv \tilde{\varepsilon}$$

So we can simulate a target Hamiltonian in the sense that the Hamiltonians are $\tilde{\varepsilon}$ close in norm and where the error $\tilde{\varepsilon}$ goes to 0 if both $\varepsilon \rightarrow 0$ and $\lambda_+ \rightarrow \infty$. Luckily, these two criteria are equivalent and upheld in this thesis, since we only choose examples for which $\lambda_- = 0, \lambda_+ = \Delta$, and $\varepsilon = O(\Delta^{-\alpha})$ for some $0 < \alpha \leq 1$.

Actually, $\alpha \leq 1$ is an upper bound on the error that comes naturally from the heuristic we use for finding H_{target} : We look at the perturbative expansion of $\Sigma(z)$, truncate it to some order in the perturbation, look at the this object to zeroth order in z and denote it H_{target} . We then compare

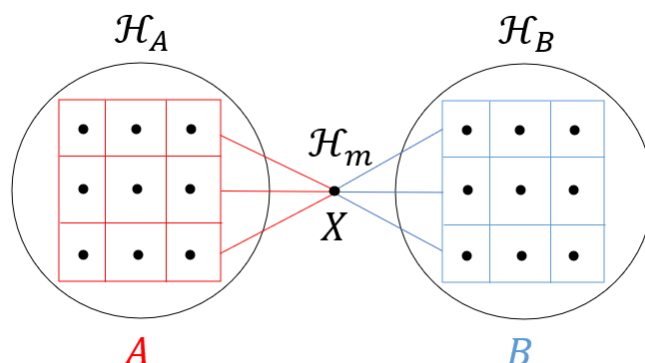


Figure 5: Schematic of the subdivision gadget. By using a simulator Hamiltonian that couples A and B to X_m , we get a virtual interaction between system \mathcal{H}_A and \mathcal{H}_B as a second order effect. Notice that both A and B should be more than 1-local if the gadget should simulate a target Hamiltonian of higher locality than the simulator.

the operator H_{target} term by term to the operator-valued function $\Sigma(z)$, which consists of terms proportional to $\frac{V_{++}^{n-1}}{(z-\Delta)^n}$. By demanding that H_{target} is independent of Δ and since H_{target} is a constant in z we get from the Laurent series of any such fraction that there will be an error from a term proportional to $\frac{z}{\Delta}$. We will further discuss this with the first example of a gadget in the next section with the conclusion that an error scaling of $\varepsilon = O(\Delta^{-1})$ is in general optimal.

We will now introduce the two archetypal examples of the perturbative gadget in the literature both proposed in [24].

4.1.1 Subdivision Gadget

Imagine we have a system containing subsystems \mathcal{H}_A , \mathcal{H}_B and an ancilla qubit \mathcal{H}_m and would like to simulate the effective interaction:

$$H_{\text{target}} = A \otimes B$$

Where A acts on \mathcal{H}_A and B acts on \mathcal{H}_B . We should think of both of these operators to be at least 2-local for the construction to be feasible. We will now construct a perturbative gadget that simulates this interaction via a coupling to an ancilla qubit as shown in figure 5.

Mathematically, we will use a simulator Hamiltonian of the form:

$$H_{\text{sim}} = H_0 + V$$

With unperturbed Hamiltonian:

$$H_0 = \Delta |1\rangle \langle 1|_m$$

And perturbation:

$$V = \sqrt{\frac{\Delta}{2}}(B - A) \otimes X_m + \frac{1}{2}(A^2 + B^2)$$

Notice that if A is k -local and B is k' -local, this perturbation is $(\max(k, k') + 1)$ -local. We get that the projections of the operators become:

$$\begin{aligned} (H_0)_{--} &= 0, & (H_0)_{++} &= \Delta N_m^z \\ V_{--} &= \frac{1}{2}(A^2 + B^2) \otimes |0\rangle \langle 0|_m, & V_{++} &= \frac{1}{2}(A^2 + B^2) \otimes |1\rangle \langle 1|_m \\ V_{+-} &= (V_{-+})^\dagger = \sqrt{\frac{\Delta}{2}}(B - A) |1\rangle \langle 0|_m \end{aligned}$$

So the self-energy is:

$$\begin{aligned} \Sigma(z) &= (H_0)_{--} + V_{--} + \frac{V_{-+}V_{+-}}{z - \Delta} + \frac{V_{-+}V_{++}V_{+-}}{(z - \Delta)^2} + \dots \\ &= 0 + \frac{1}{2}(A^2 + B^2) |0\rangle \langle 0|_m + \frac{\Delta}{2(z - \Delta)}(B - A)^2 |0\rangle \langle 0|_m + \frac{\Delta}{4(z - \Delta)^2}(B - A)^2(A^2 + B^2) |0\rangle \langle 0|_m + \dots \end{aligned}$$

We will analyse the expression via the following Laurent series which we will use time and time again in this thesis:

$$\frac{\Delta^\alpha}{(z - \Delta)^\beta} = (-1)^\beta \Delta^{\alpha - \beta} \left(1 - \beta \frac{z}{\Delta} + \beta(\beta + 1) \left(\frac{z}{\Delta}\right)^2 + O\left(\left(\frac{z}{\Delta}\right)^3\right) \right) \quad (6)$$

If we do the Laurent series of the second order term, we get:

$$\frac{\Delta}{2(z - \Delta)}(B - A)^2 |0\rangle \langle 0|_m = -\frac{1}{2}(B^2 + A^2 - 2AB) \left(1 - \frac{z}{\Delta} + O\left(\frac{z}{\Delta}\right)^2 \right) |0\rangle \langle 0|_m$$

And we see that the first order term $\frac{1}{2}(A^2 + B^2) |0\rangle \langle 0|_m$ cancels partially with this expression to constant order in z . By doing the Laurent series on the third order term, we get:

$$\frac{\Delta}{4(z - \Delta)^2}(B - A)^2(A^2 + B^2) |0\rangle \langle 0|_m = \frac{1}{4}(B - A)^2(A^2 + B^2) \left(\frac{1}{\Delta} + O\left(\frac{z}{\Delta^2}\right) \right) |0\rangle \langle 0|_m$$

Higher order terms in the geometric series will constitute a smaller error by the condition $\Delta \geq \frac{\|V\|}{2}$ which we enforce such that the perturbation doesn't break down. Thus, we produce the total self-energy:

$$\Sigma(z) = A \otimes B \otimes |0\rangle \langle 0|_m + O\left(\frac{z}{\Delta}\right)$$

And by Theorem 1 and its preceding Lemma, the low-energy part of H_{sim} simulates the spectrum of $H = H_{\text{target}} \otimes |0\rangle \langle 0|_m$ up to error $\varepsilon = O(\Delta^{-1})$ and $(H_{\text{sim}})_{\leq \Delta}$ is $\tilde{\varepsilon}$ close to H in 2-norm.

Notice here what we talked about in section 4.1: We can at best take care of the constant order of z in H_{target} , so the first order term of z in $\Sigma(z)$ must always be interpreted as an error. If the target Hamiltonian should be independent of Δ , this means that the first order term in z always will be of the form $\beta \frac{z}{\Delta}$ for some $\beta \in \mathbb{R}$, so an error of $O(\Delta^{-1})$ will in general always be present. Subsequently, the error of the subdivision gadget scales as well as possible with respect to the heuristic we use.

The conclusion of the gadget is as follows: If A and B were k -local operators their product is $2k$ -local but can be simulated by two $(k+1)$ -local terms and two k -local terms. Hence the subdivision gadget simplifies a system of locality $2k$ to $k+1$. Likewise, If $A \otimes B$ had locality $2k+1$, the gadget simplifies the interaction to locality $k+2$. Subsequently, we conclude that the subdivision gadget simulates a k -local interaction via a $(\lceil \frac{k}{2} \rceil + 1)$ -local interaction. This gadget can be used iteratively n times to simulate something like a 2^n -local Hamiltonian but at the requirement of energy gaps Δ_n that also scale exponentially [6], which makes the construction unfeasible in regards to simulating Hamiltonians of arbitrary locality. The gadget can also be applied to sums of Hamiltonians but at the cost of the error growing with the number of terms in the Hamiltonian [6].

Originally this gadget was used to show universal simulability of 3-local Hamiltonians. In order to get the stronger result that 2-local Hamiltonians are universal simulators, one needs the other archetypal example of a gadget called the 3-to-2-gadget, which we'll present now.

4.1.2 3-to-2 Gadget

In a situation like the one for the subdivision gadget but with systems $\mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_C$ and ancilla qubit \mathcal{H}_m , we want to simulate an effective interaction between the three systems $\mathcal{H}_A, \mathcal{H}_B$ and \mathcal{H}_C :

$$H_{\text{target}} = A \otimes B \otimes C$$

We will think of these three interactions as 1-local but they don't have to be in the following simulation.

This can be done via the Perturbative gadget using the simulator:

$$H_{\text{sim}} = H_0 + V$$

With unperturbed Hamiltonian:

$$H_0 = \Delta |1\rangle \langle 1|_m$$

And 2-local perturbation:

$$V = \overbrace{\frac{\Delta^{2/3}}{\sqrt{2}}(B+A) \otimes X_m}^{V_{\text{jump}}} + \overbrace{\Delta^{2/3} C \otimes N_m^z}^{V_{\text{high}}} + \overbrace{\frac{\Delta^{1/3}}{2}(A+B)^2 - \frac{1}{2}(A^2+B^2)C}^{V_{\text{counter}}}$$

Where the index m signifies the ancilla qubit. We see that $V_{+-} = (V_{-+})^\dagger = (V_{\text{jump}})_{+-}$, $V_{++} = (V_{\text{high}} + V_{\text{counter}})_{++}$, $V_{--} = (V_{\text{counter}})_{--}$. The first term of the perturbation makes the ancilla qubit jump from low- to high-energy, the second term only acts in the high-energy subspace of the ancilla qubit and the last two terms are needed in order to cancel unwanted terms in the self-energy.

In total, the self-energy to third order in the potential becomes:

$$\begin{aligned}\Sigma(z) &= (H_0)_{--} + V_{--} + \frac{V_{-+}V_{+-}}{z - \Delta} + \frac{V_{-+}V_{++}V_{+-}}{(z - \Delta)^2} + \dots \\ &= 0 + V_{\text{counter}} |0\rangle \langle 0|_m + (B + A)^2 \frac{\Delta^{4/3}}{2(z - \Delta)} |0\rangle \langle 0|_m + (B + A)^2 C \frac{\Delta^2}{2(z - \Delta)^2} |0\rangle \langle 0|_m \\ &\quad + (B + A)^2 V_{\text{counter}} \frac{\Delta^{4/3}}{(z - \Delta)^2} |0\rangle \langle 0|_m + \dots\end{aligned}$$

We will now analyze each term by taking the Laurent-expansion of the fractions $\frac{\Delta^\alpha}{(z - \Delta)^\beta}$ with respect to z like we did in equation 6. We will refer to the different terms of the self-energy by "the n 'th order term of the self-energy", which means terms for which there are n multiples of V multiplied with each other. Of these, we will refer to the terms of their Laurent series as "the n 'th order term with respect to z ", which means that we refer to the terms of the form $\left(\frac{z}{\Delta}\right)^n$ of the Laurent series.

First, notice the first order term in the perturbation V_{counter} . We see that the $(A + B)^2$ -term of V_{counter} acts as a counter term for the second order term of the self energy and they cancel to zeroth order in z :

$$\frac{\Delta^{1/3}}{2} (A + B)^2 |0\rangle \langle 0|_m + (B + A)^2 \frac{\Delta^{4/3}}{(z - \Delta)} |0\rangle \langle 0|_m = O\left(\frac{z}{\Delta^{2/3}}\right)$$

Furthermore, the $(A^2 + B^2)C$ -term of V_{counter} kills off unwanted terms in the third order term of the self energy to zeroth order in z :

$$-\frac{1}{2} (A^2 + B^2) C |0\rangle \langle 0|_m + (B + A)^2 C \frac{\Delta^2}{2(z - \Delta)^2} |0\rangle \langle 0|_m = ABC + O\left(\frac{z}{\Delta}\right)$$

Thus, up to third order in the perturbation, the only non-zero term in the self-energy becomes $H = A \otimes B \otimes C \otimes |0\rangle \langle 0|_m$ to zeroth order in z . Now we just need to find its error.

The second order term of the self-energy with respect to the potential then has an error term of order $O(\Delta^{-2/3})$ from its Laurent series to first order in z . To third order in the self-energy, the V_{counter} -term has an error of order $O(\Delta^{-1/3})$ from its Laurent series to zeroth order in z and the $(B + A)^2 C$ -term has an error of $O(\Delta^{-1})$ to first order in z . The largest part of the fourth order term in the self-energy expansion $\frac{V_{-+}V_{++}^2V_{+-}}{(z - \Delta)^3}$ is of order $O(\Delta^{-1/3})$ to zeroth order in z . The total error scales like the worst of these, which means to order $\varepsilon = O(\Delta^{-1/3})$.

Putting all of this together, Theorem 1 and Lemma 1 says that the low-energy part of H_{sim} simulates the spectrum of $H = H_{\text{target}} \otimes |0\rangle \langle 0|_m$ up to error $\varepsilon = O(\Delta^{-1/3})$ and the norm difference

between the low-energy part of the simulator and the target Hamiltonian is $\tilde{\varepsilon}$.

This is the final gadget needed to prove universal simulability of the 2-local Hamiltonian in the context of the k -local-Hamiltonian problem. In regards to locality, the result of going from a 3-local Hamiltonian to a 2-local is a lot less impressive than going from k to $\lceil \frac{k}{2} \rceil + 1$ as we do in the subdivision gadget. On the other side, this jump is very needed if all one can implement are 2-local interactions and want to create a k -local Hamiltonian.

In the context of universal gate sets, this is also in strong analogue to the universality of 2-local gates. We know that any unitary can be simulated via CNOT- and on-site-interactions. The universal simulability of 2-local Hamiltonians might produce a stronger result in the context of simulations of gates, since this shows that the Toffoli-interaction can be simulated arbitrarily well with just 2-local time-independent Hamiltonians. This warrants a hope that one can find an even simpler universal gate set than the Hadamard and the Toffoli, if the Toffoli can be simulated by a small amount of easily implementable 2-local interactions. If the implementation is easy enough, one could hope that it might even be a more feasible set of interactions than the CNOT and 1-qubit gate set.

In regards to this Master thesis, this is very much where we started our attempt to create a gadget which could simulate the Toffoli gate with as little local complexity as possible. That is also the context with which we will introduce our novel perturbative gadgets in the following sections.

4.1.3 Full geometric series

In the Perturbative gadget, each term in the geometric series of the self-energy gets expanded as a Laurent series like that of equation 6. In order to simulate a target Hamiltonian, one then needs to look at this expansion to constant order in z to realize which target Hamiltonian we simulate. Typically, the geometric series has been truncated at the order of locality we wanted our target interaction to have and the rest of the sum have been perceived as error terms. Here, I would like to show examples of scenarios for which one can instead utilize the entire geometric series to simulate a target Hamiltonian. The strength of this is that the error will scale as good as theoretically possible, that is as $\varepsilon = O(\Delta^{-1})$ like we discussed in section 4.1. The hard part is then to see which scenarios this is actually possible for.

Invertible C. The first example we'll present is very similar to the 3-to-2-gadget. One can make a stronger version of the 3-to-2-gadget with lesser connectivity and to higher precision, if one assumes C to be invertible and to have the property that $\|\mathbb{1} - C^{-1}\| < \frac{1}{2}$. By choosing $D = \mathbb{1} - C^{-1}$, we can simulate the interaction:

$$H_{\text{target}} = (A + B)^2 C$$

With simulator:

$$H_{\text{sim}} = H_0 + V$$

Unperturbed Hamiltonian:

$$H_0 = \Delta N_m^z$$

And perturbation

$$V = \Delta^{1/2}(A + B) \otimes X_m + \Delta D \otimes |1\rangle \langle 1|_m$$

Then the self-energy becomes:

$$\begin{aligned} \Sigma(z) &= V_{-+} \sum_{n=0}^{\infty} \frac{(V_{++})^n}{(z - \Delta)^{n+1}} V_{+-} = (A + B)^2 \sum_{n=0}^{\infty} \frac{\Delta^{n+1}}{(z - \Delta)^{n+1}} D^n \otimes |0\rangle \langle 0|_m \\ &= (A + B)^2 \frac{1}{1 - D} \otimes |0\rangle \langle 0|_m + O\left(\frac{z}{\Delta}\right) = (A + B)^2 C \otimes |0\rangle \langle 0|_m + O(\Delta^{-1}) \end{aligned}$$

Notice that the assumption that $\|D\| < \frac{1}{2}$ is needed for the geometric series to converge, but also because Theorem 1 demands $\|V\| \leq \frac{\Delta}{2}$. This norm bound on D implies that $\frac{2}{3} < \|C\| < 2$. Typically in quantum mechanics, interactions are physically equivalent under scaling $C \rightarrow cC$, $c \in \mathbb{R} \setminus \{0\}$ and shift $C \rightarrow C + c\mathbb{1}$, $c \in \mathbb{R}$ but shifts will in this example change global dynamics $A \otimes B \otimes C \rightarrow A \otimes B \otimes C + cA \otimes B \otimes \mathbb{1}$ and therefore won't produce the same physics. Thus either the upper or lower norm bound on C can be fulfilled by scaling, but we have no promise that the other bound is achievable.

As long as C is invertible and the bound on D is true, the simulator Hamiltonian simulates the Hamiltonian $H = H_{\text{target}} \otimes |0\rangle \langle 0|_m$ by Theorem 1. Like for the subdivision gadget, this error is optimal since Theorem 1 has to hold for all relevant z 's meaning that the self-energy can at best be fixed to constant order in z .

Idempotence If instead both A, B and C have the property that they square to themselves then we have a situation like that of the Toffoli interaction, where the target Hamiltonian is the tensor product of three projections. Then we can simulate the interaction:

$$H_{\text{target}} = -A \otimes B \otimes C$$

To optimal error via a 2-local simulator Hamiltonian by using the full geometric series-construction. We apply the simulator:

$$H_{\text{sim}} = H_0 + V$$

With unperturbed Hamiltonian:

$$H_0 = \Delta |1\rangle \langle 1|_m$$

And perturbations:

$$V = V_{\text{target}} + V_{\text{counter}}$$

Of the form:

$$V_{\text{target}} = \sqrt{\frac{\Delta}{2}} \left(A + B - \frac{1}{2} \right) \otimes X_m - \frac{\Delta}{2} C \otimes |1\rangle \langle 1|_m$$

$$V_{\text{counter}} = AB + \frac{1}{8} + \frac{1}{8} C \otimes |0\rangle \langle 0|_m$$

By the idempotence of A and B , we get that:

$$V_{-+} V_{+-} = \Delta \left(AB + \frac{1}{8} \right)$$

In this scenario, the geometric series of the self-energy becomes:

$$\begin{aligned} \Sigma(z) &= (H_0)_{--} + V_{--} + \frac{V_{-+} V_{+-}}{(z - \Delta)} + \sum_{n=1}^{\infty} \frac{V_{-+} V_{++}^n V_{+-}}{(z - \Delta)^{n+1}} \\ &= (V_{\text{counter}})_{--} + \left(AB + \frac{1}{8} \right) \frac{\Delta}{z - \Delta} \otimes |0\rangle \langle 0|_m - \left(AB + \frac{1}{8} \right) C \sum_{n=2}^{\infty} \frac{1}{2^{n-1}} \frac{\Delta^n}{(\Delta - z)^n} \otimes |0\rangle \langle 0|_m + V_{\text{error}} \end{aligned}$$

Where V_{error} is of the form:

$$V_{\text{error}} = \sum_{n=0}^{\infty} \frac{V_{-+} V_{++}^n V_{+-}}{(z - \Delta)^{n+1}} - \left(AB + \frac{1}{8} \right) \frac{\Delta}{z - \Delta} \otimes |0\rangle \langle 0|_m - \left(AB + \frac{1}{8} \right) C \sum_{n=2}^{\infty} \frac{1}{2^{n-1}} \frac{\Delta^n}{(\Delta - z)^n} \otimes |0\rangle \langle 0|_m$$

That is "the rest" of the expansion that we haven't explicitly written out in the self-energy above. Notice that every term in the infinite series of V_{error} is at least of order $O(\Delta^{-1})$. This is because it is constructed as a sum of the form $V_{-+}^n - (V_{\text{target}})_{++}^n = (V_{\text{target}} + V_{\text{counter}})_{++}^n - (V_{\text{target}})_{++}^n$ for all positive integers n . Expanding the parenthesis, each term will at most have weight Δ^{n-1} since only $(V_{\text{target}})_{++}^n$ has weight Δ^n . Thus $V_{-+}(V_{++}^n - (V_{\text{target}})_{++}^n)V_{+-}$ consists of terms of at most order Δ^n and will get suppressed by the division with $(z - \Delta)^{n+1}$ in the geometric series to give $O(\Delta^{-1})$ altogether.

By expanding the rest of the fractions in the self-energy into their Laurent series in z (like in equation 6), we get to zeroth order in z that the infinite sum becomes a geometric series in the number $\frac{1}{2}$, which sums to 1. The low-energy-projection of the counter term cancels the second order term and the infinite series multiplied onto $\frac{1}{8}C$ to zeroth order in z . In conclusion, to constant order in z we get that $\Sigma(z) = -A \otimes B \otimes C + O(\Delta^{-1})$ and by Theorem 1, we simulate the Hamiltonian $H_{\text{target}} = -A \otimes B \otimes C$ to error $\varepsilon = O(\Delta^{-1})$. This class of Hamiltonians include the Toffoli-interaction up to a sign, but this just corresponds to going backwards in time instead of forward. After waiting $t = \pi$ seconds, we still get a Toffoli-gate.

4.1.4 Direct k -local Gadget

Both the 3-to-2 and the subdivision gadgets work in some sense by coupling the jumping in energy of an ancilla qubit with an interaction to another system. The perturbative expansion of the self-energy corresponds to propagation up and down in energy of the ancilla qubit, which instigates couplings between different systems. The natural way to think about this as a physicist is in the language of Feynman Diagrams and propagations of virtual particles that mitigates interaction that weren't there before.

As a sort of generalization of this idea, one can instead use an ancilla qudit of local dimension k for the construction. Then one can couple interactions between the systems through excitations that are independent. To make this idea more concrete: If one has an ancilla qudit with k energy levels, one can simulate the interaction:

$$H_{\text{target}} = \bigotimes_{j=0}^{k-1} A_j$$

Via the Perturbative gadget with simulator Hamiltonian:

$$H_{\text{sim}} = H_0 + V + V_{\text{counters}}$$

A non-perturbed Hamiltonian:

$$H_0 = \Delta \sum_{j=1}^{k-1} |j\rangle \langle j|$$

And 2-local perturbation:

$$V = \frac{\Delta^\alpha}{\sqrt{2}^k} \sum_{j=0}^{k-1} A_j \otimes (|j\rangle \langle j+1| + |j+1\rangle \langle j|)$$

Where V_{counter} contains some counter terms that depend on your concrete system, which we'll come back to characterizing. In the perturbation, the quantum numbers should be interpreted modulo k , so $|k\rangle = |0\rangle$ and the parameter α is $\alpha = 1 - \frac{1}{k}$.

One can intuitively understand why this works: The perturbation of the self-energy couples factors A_j to the transition of state $|j\rangle$ to $|j+1\rangle$ on the ancilla qudit. Thus, the k 'th order term $V_{-+} V_{++}^{k-2} V_{+-}$ in the self-energy will contain a term where the qudit has transitioned to every state once before ending back at $|0\rangle_m$, subsequently adding a coupling of each A_j on the way. This corresponds to simulating our wanted target Hamiltonian.

This intuition also explains why we need a counter term to cancel unwanted interactions. The perturbation corresponds to "jumps" up or down the ladder of states of the qudit. With a fixed amount of jumps there are many ways one can transition up and down the ladder of states and end back in $|0\rangle_m$. Any such jumping scheme produces a term in the self-energy which couples

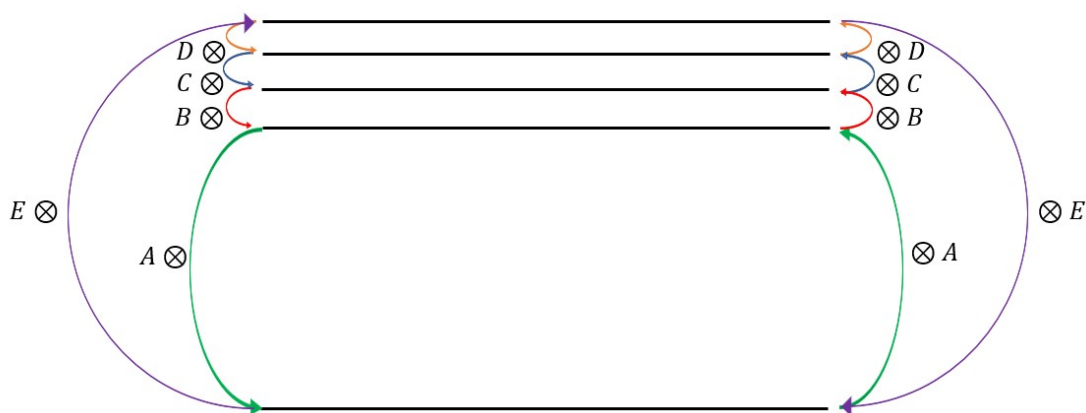


Figure 6: Graphical Representation of the direct k-local Gadget. The jumping of energy levels on the ancilla qubit corresponds to coupling with an interaction on the rest of the system. In order to survive in the self-energy perturbative expansion, the "jumping up and down the ladder" needs to end up at the ground state again, which limits the possible ways to couple the systems at a fixed perturbation order.

each A_j for indexes j 's that correspond to the indexes one has transitioned between in the jumping scheme (See figure 6 for a schematic of this intuition).

The necessity of the counter term V_{counter} to get the bare k -local interaction, also stems from the fact that there will always be non-zero contributions from at least the even terms up to order k . That even terms in the expansion of lower order than the locality we attempt to simulate can't be 0 is a general feature of the Perturbative gadget, which we'll show now. For any perturbation V , we have that the $2n + 2$ 'th order term is proportional to:

$$V_{-+}(V_{++})^{2n}V_{+-} = S^\dagger S$$

With $S \equiv (V_{++})^n V_{+-}$. An operator of the form $S^\dagger S$ is 0 iff. $S = 0$, since $S^\dagger S$ is a positive semi-definite operator. Any term of higher order in the geometric series of the self-energy will have the form:

$$V_{-+}(V_{++})^{m+2n}V_{+-} = S^\dagger (V_{++})^m S$$

Which will be 0 if S was 0. Thus, if any even order terms of the self-energy is zero, we force every term of higher order to also be zero.

One should think of V_{counter} as consisting of all the unwanted "jumping" terms. If we wanted to simulate a target Hamiltonian that is the tensor product of k on-site terms, V_{counter} would get a

contribution for every even order term all the way up to k by the previous argument. Sadly it would also get many other contributions which one would like to characterize. For instance, If k is even you can't jump up and down the ladder and end at position $|0\rangle$ again in an odd amount of jumps, so every odd term would die. If k is odd, you can get back and forth on an odd amount of jump, so the odd terms live.

Naively, one could think that we could just simulate a target Hamiltonian that contains all these unwanted jumping terms as part of what one attempts to simulate. This is regrettably not optimal. The reason is that the norm-bound on the self-energy of Theorem 1 has to hold for all $z \in [\min \text{Spec}(H_{\text{target}}), \max \text{Spec}(H_{\text{target}})]$. If we don't kill off these terms, $\|H_{\text{target}}\|$ can grow to order Δ^γ for some $\gamma > 0$ which implies that z can as well. We recall what the general Laurent series we use time and time again looks like:

$$\frac{\Delta^\alpha}{(z - \Delta)^\beta} = (-1)^\beta \Delta^{\alpha-\beta} \left(1 - \beta \frac{z}{\Delta} + \beta(\beta+1) \left(\frac{z}{\Delta}\right)^2 + \dots \right)$$

Not killing off the counter terms will mean that z can run up to Δ^γ , implying that the first order term of the Laurent series will become an error term of size $\Delta^{\alpha-\beta+\gamma-1}$ instead of $\Delta^{\alpha-\beta-1}$ as we would without a Δ -dependence of H_{target} . Thus, one really needs to kill off these terms in order to get feasible errors, but as no fixed method will guarantee their demise, one needs to construct counter terms dependent on the concrete problem.

In general, this construction leaves a lot to be wanted. We have argued that it is impossible to get rid of V_{counter} for $k > 2$, so this method will always produce unwanted counter terms. Another point of criticism of the gadget is that if one analyzes its errors, one finds that it scales like $O(\Delta^{-\frac{1}{k}})$. This is rather poor convergence relatively to the other gadget constructions. For clarification, we will in the following section apply this construction for a qudit of $k = 3$ energy levels, where we also construct the needed counter-terms for the gadget.

Example of direct 3-local Gadget

As an example of the above, imagine that one would want to simulate the interaction

$$H_{\text{target}} = A \otimes B \otimes C$$

just like in the 3-to-2-gadget. Then the direct 3-local gadget provides a method to do so with a lower connectivity than the 3-to-2-gadget.

Just like above, we make the simulator:

$$H_{\text{sim}} = H_0 + V + V_{\text{counter}}$$

With unperturbed Hamiltonian:

$$H_0 = \Delta \sum_{j=1}^2 |j\rangle \langle j|_m = \Delta |1\rangle \langle 1|_m + \Delta |2\rangle \langle 2|_m$$

2-local perturbation:

$$V = \frac{\Delta^\alpha}{\sqrt{2}} A \otimes (|0\rangle\langle 1|_m + |1\rangle\langle 0|_m) + \Delta^\gamma C \otimes (|1\rangle\langle 2|_m + |2\rangle\langle 1|_m) + \frac{\Delta^\alpha}{\sqrt{2}} B \otimes (|0\rangle\langle 2|_m + |2\rangle\langle 0|_m)$$

And 2-local counter term of the form:

$$V_{\text{counter}} = \frac{\Delta^{2\alpha-1}}{2} (A^2 + B^2) |0\rangle\langle 0|_m$$

Notice that we don't choose the constant scaling $\Delta^{-1/3} = \Delta^{2/3}$ as the recipe of the previous section would have us do, but instead chose unknown exponents α and γ that we will determine later for minimum error of the simulation. Notice also that we switched the weights in front of each term a bit around such that the self-energy is easier to calculate.

The self-energy to fourth order becomes:

$$\begin{aligned} \Sigma(z) &= (H_0)_{--} + V_{--} + \frac{V_{-+}V_{+-}}{(z-\Delta)} + \frac{V_{-+}V_{++}V_{+-}}{(z-\Delta)^2} + \frac{V_{-+}V_{++}^2V_{+-}}{(z-\Delta)^3} + \dots \\ &= 0 + \frac{\Delta^{2\alpha-1}}{2} (A^2 + B^2) \otimes |0\rangle\langle 0|_m + \frac{A^2 + B^2}{2} \otimes |0\rangle\langle 0|_m \frac{\Delta^{2\alpha}}{(z-\Delta)} + A \otimes B \otimes C \otimes |0\rangle\langle 0|_m \frac{\Delta^{2\alpha+\gamma}}{(z-\Delta)^2} \\ &\quad + \frac{1}{2} (A^4 + B^4 + 2A^2B^2) \otimes |0\rangle\langle 0|_m \frac{\Delta^{4\alpha}}{(z-\Delta)^3} + \frac{1}{2} (A^2C^2 + B^2C^2) \otimes |0\rangle\langle 0|_m \frac{\Delta^{2\alpha+2\gamma}}{(z-\Delta)^3} + \dots \end{aligned}$$

We analyze the Laurent series in z for each term. The first order term that comes from V_{counter} counters the second order term in the self-energy to constant order in z . We see that the third order term gives us the target Hamiltonian to constant order in the Laurent series but only if $2\alpha + \gamma = 2$. Under this assumption, the remaining terms represent errors. Thus, by expanding the second and third order terms of the self-energy to first order in z and the fourth order terms of the self-energy to constant order in z , we get that the four leading orders of errors are:

$$\begin{aligned} \Sigma(z) - A \otimes B \otimes C \otimes |0\rangle\langle 0|_m &= z\Delta^{2\alpha-2} \frac{A^2 + B^2}{2} \otimes |0\rangle\langle 0|_m + z\Delta^{2\alpha+\gamma-3} ABC \otimes |0\rangle\langle 0|_m \\ &\quad + \frac{1}{2} \Delta^{4\alpha-3} (A^4 + B^4 + 2A^2B^2) \otimes |0\rangle\langle 0|_m + \frac{1}{2} \Delta^{2\alpha+2\gamma-3} \otimes |0\rangle\langle 0|_m + \dots \end{aligned}$$

The left out terms in the self-energy will decay faster than the terms explicitly written out above by the fact that the perturbation doesn't break down ($\Delta \geq \frac{\|V\|}{2}$). Therefore the total error grows like the worst of these four terms. By utilizing that $2\alpha + \gamma = 2$, we get that the exponents of Δ respectively become $-\gamma, -1, 1 - 2\gamma, \gamma - 1$. These four terms are simultaneously minimized when $\gamma = \frac{2}{3}$, implying $\alpha = \frac{2}{3}$. Therefore, the optimal error of this gadget scales as $\varepsilon = O(\Delta^{-1/3})$ which is exactly the same as for the 3-to-2-gadget.

It might seem like we don't win anything via this construction in comparison to the 3-to-2-gadget but there is one clear difference in the outcome: The direct 3-local gadget only needs strong control onto the ancilla qubit meaning that it is not necessary to have connectivity between systems \mathcal{H}_A , \mathcal{H}_B and \mathcal{H}_C as is needed for the 3-to-2-gadget. If we instead assumed full 2-local

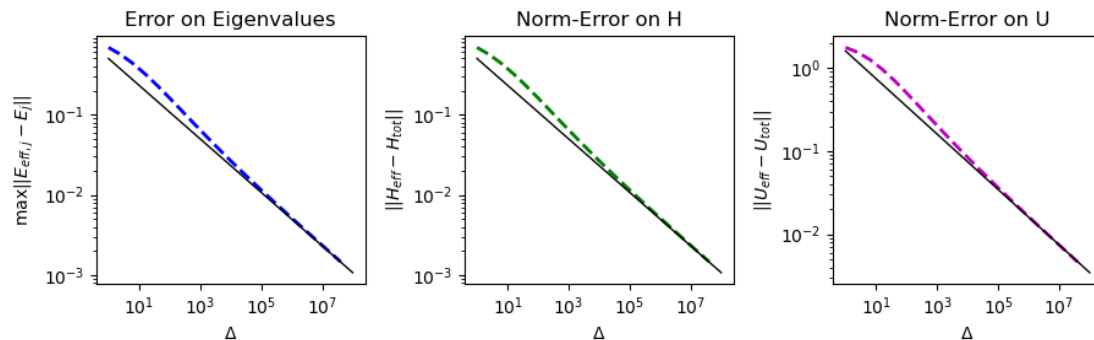


Figure 7: Simulation of a Toffoli via the direct-3-local gadget, represented via the maximum difference in eigenvalues, the distance in 2-norm of interactions and the distance of 2-norms of the time-evolutions after waiting $t = \pi$ time plotted on log-log-axes (dotted lines). We have furthermore plotted linear functions that have a slope of $-\frac{1}{3}$ to show the asymptotic behaviour (full drawn lines). The tails of the three plots have been fitted to linear functions, and produce slopes that lie in the interval $a \in [-0.346307, -0.346287]$.

connectivity we could add more counter-terms to the perturbation to make the error smaller. Sadly this process is non-trivial, as counter terms would either have high locality by being coupled to $|0\rangle\langle 0|_m$ or introduce a non trivial contribution to V_{++} , which one would need to subtract again to minimize error. All in all, this produces an iterative process that exactly corresponds to the adding of counter terms in Feynman Diagram renormalization, which is a whole literature in and on itself.

In the next section, we will implement the constructions we have created so far in Python and numerically simulate the errors on them.

4.1.5 Simulations of error on Toffoli

Every attempt we've made at characterizing the error of our constructions has been bounded as functions of Δ but only asymptotically. We learn from our analysis that the error scales like some order $\varepsilon = O(\Delta^{-\gamma})$ for positive γ but for any finite Δ , what is actually this error?

We will in this section simulate the Toffoli interaction, that is $A = N_1^z$, $B = N_2^z$, $C = N_3^x$. We will do so first with the direct-3-local gadget and then with the full-geometric-series-gadget. We will look at all three notions of simulation introduced in section 2: How close the eigenvalues of the simulator and the target Hamiltonian are, how far apart they are in norm and how far their time-evolutions are from each other in norm.

Direct-3-Local Gadget: By simulating the Toffoli via the direct-3-local gadget, we get the plots of figure 7. We find that the behavior of the error is close to the asymptotic description:

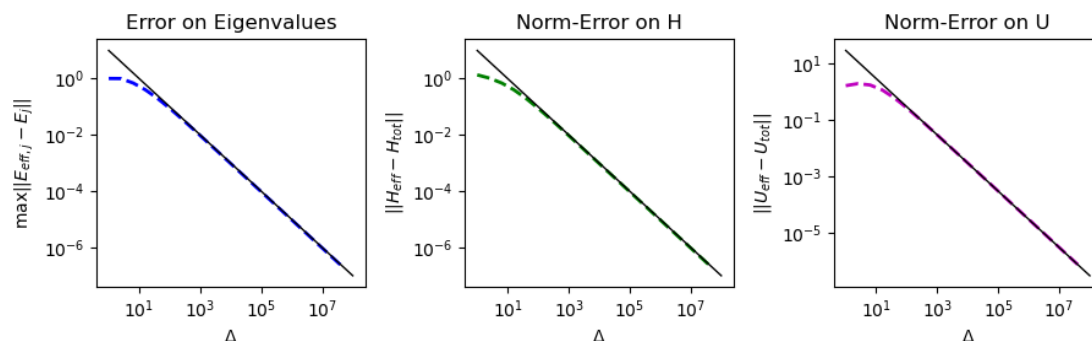


Figure 8: Simulation of a Toffoli via the full geometric series gadget, represented via the maximum difference in eigenvalues, the distance in 2-norm of interactions and the distance of 2-norms of the time-evolutions after waiting $t = \pi$ time plotted on log-log-axes (dotted lines). We have furthermore plotted linear functions that have a slope of -1 to show the asymptotic behaviour (full drawn lines). The tails of the three plots have been fitted to linear functions, and produce slopes between $a \in [-1.00029, -0.99995]$.

It scales like $\sim \Delta^{-0.3463}$, which is rather close to the theoretical $\varepsilon = O(\Delta^{-1/3})$.

Full Geometric Series: By simulating the Toffoli via the full-geometric-series gadget, we get the plots of figure 8. We see that the behavior of the error is close to the asymptotic description: It scales like $\sim \Delta^{-1.0001}$, which is really close to the theoretical prediction of $\varepsilon = O(\Delta^{-1})$.

4.1.6 Adding an error term

We have now introduced many different gadget constructions, both those that are common in the literature like the subdivision and the 3-to-2-gadget and some novel gadgets constructed for this thesis like the direct-k-local-gadget and the full-geometric-series-gadget. They work as strong building blocks for simulating target Hamiltonians of high locality but every construction so far has focused only on simulating operators that can be written as product operators. It is still unclear in this context how one would simulate a Hamiltonian that is the sum of two product operators and that is what we will discuss in this section.

In the literature [6], there are examples of analyses of how the error of the Perturbative gadget scales when one adds an extra term outside the perturbation, that is:

$$H_{\text{sim}} = H_0 + V + H_{\text{extra}}$$

We think of the first two terms as the Hamiltonian we want to gadgetize and the last one as a term we would like not to tamper with. Mathematically, one would in this scenario attempt to

simulate the target Hamiltonian:

$$H_{\text{target}} = \tilde{H}_{\text{target}} + H_{\text{extra}}$$

Where $\tilde{H}_{\text{target}}$ was the target Hamiltonian one would simulate from the Hamiltonian $H_{\text{sim}} = H_0 + V$.

By interpreting H_{extra} as part of the unperturbed Hamiltonian, this won't change the form of the perturbative expansion, but it will change the low- and high-energy-subspaces, so P_- and P_+ will differ from before. Examples in the literature that do this, prove the applicability of the Perturbative gadget when the form of H_{extra} is known, like it has been proven for the subdivision gadget applied in parallel [6]. There sadly aren't strong results of under which conditions $\|H_{\text{sim}} - H_{\text{extra}}\|$ goes to zero or how the behavior of this convergence would be in all generality. This makes it unfeasible to make arbitrary constructions of the above form.

This could seem like a meaningless loss, but it means that it is hard to know how well it would work to put two of these gadgets in parallel, that is if we implemented the Hamiltonian:

$$H_{\text{sim}} = \sum_i H_{i,\text{sim}}$$

for which we have a promise that each $H_{i,\text{sim}}$ simulates the interaction $H_{i,\text{target}}$ up to error $\varepsilon_i = O(\Delta^{-\alpha_i})$ for some exponents α_i . The fact that it is hard to bound extra terms means that in general, it is hard to state exactly how the error of the simulation of $H_{\text{target}} = \sum_i H_{i,\text{target}}$ scales as a function of the individual gaps. Thus, this framework doesn't warrant easy constructions for how one can make arbitrary high local simulations in a controlled manner, and thus stops its natural usage in the context of physical implementations at the level of small toy-constructions like the ones in this thesis until there are stronger results on the convergence of parallelizations work.

4.2 Logical Gadgets

The Perturbative gadget paved the way for a very new way to think about analogue Hamiltonian simulation and as we showed in the previous section, it has the capacity to simulate many different classes of Hamiltonians. One limitation of this approach is its ability to simulate target Hamiltonians only in an approximate or perturbative manner. On the other hand, we have the Logical gadget, originally proposed in [4] and explored more in depth in [6]. The Logical gadget is in strong contrast to the gadgets proposed by [18]: Where the Perturbative gadget makes use of the self-energy to approximate dynamics of a Hamiltonian, the Logical gadget works exact and with no error as long as there is a promise of being in the low-energy-space. In the following sections, we will look at the AND-logic gadget introduced in [4] and construct novel Logical gadgets ourselves.

The Logical gadget is a tool to simulate Hamiltonians that consists of tensor products of projections. By interpreting projections as binary logical variables, we can use standard methods in the theory of polynomial unconstrained binary optimization (PUBO) to minimize the locality of the problem. The interpretation of projections as binary variables must be understood in the sense that the projections hold different binary values in different subspaces that they act on: In the subspace that the projections has support on, the projection is interpreted as a binary 1, and on its kernel the projection is interpreted as a binary 0.

In the framework of Logical gadgets, we add a penalization Hamiltonian, whose low-energy-subspace exactly corresponds to the validity of a logical statement we would like to be true. For instance, observe the following penalty Hamiltonian on two target qubits and an ancilla qubit:

$$H_{\text{AND}} = \Delta(3N_m - 2N_1N_m - 2N_2N_m + N_1N_2) \quad (7)$$

Where N_k is the projector onto a 1-dimensional subspace acting on the k 'th qubit and Δ is a gap parameter. This Hamiltonian is diagonal in the basis spanned by the vectors that define the 1-dimensional projectors. Table 2 shows the energies of possible states in this construction.

It is evident from Table 2 that this Hamiltonian has a 0-energy-subspace of states that are characterized by the logical statement " $N_m = N_1 \wedge N_2$ " when viewed as logical variables. Therefore, the promise of being in the low-energy-subspace equivalently becomes a promise that this logical statement is fulfilled.

By choosing $N_1 = \neg M_1$ and $N_2 = \neg M_2$ as logical variables in the above construction, that is by choosing $N_1 = 1 - M_1$ and $N_2 = 1 - M_2$ as projections, the penalty Hamiltonian has a subspace that is characterized by the logical statement " $N_m = \neg M_1 \wedge \neg M_2 = \neg(M_1 \vee M_2) \equiv \text{NOR}(M_1, M_2)$ ". This means that through 2-local interactions, one can make a low-energy-subspace which is equivalent to a NOR-statement. By the logical universality of the NOR-gate, one should be able to make a multitude of logical statements as the low-energy subspace of com-

Eigenstates	Energies of H_{penalty}
$ 0_1 0_2 0_m\rangle$	0
$ 0_1 0_2 1_m\rangle$	3Δ
$ 0_1 1_2 0_m\rangle$	0
$ 0_1 1_2 1_m\rangle$	Δ
$ 1_1 0_2 0_m\rangle$	0
$ 1_1 0_2 1_m\rangle$	Δ
$ 1_1 1_2 0_m\rangle$	Δ
$ 1_1 1_2 1_m\rangle$	0

Table 2: Energies of the different eigenstates of H_{penalty} . Here a logical 0_k means that $N_k |0\rangle_k = 0$ and a logical 1_k means that $N_k |1\rangle_k = |1\rangle_k$.

binations of penalization Hamiltonians.

Thus, these "Logical gadgets" are a method for transforming formulations of logical statements on one or more ancilla qubits into problems of low-energy-subspaces of Hamiltonians. The strength of the method comes from the fact that a logical statement that consists of many logical literals can be made with a Hamiltonian that has a lower locality than the statement has literals. This works as a way to lower the locality-complexity of the problem and makes it easier to implement or solve.

We will now introduce a gadget that is introduced in [4], which works as an extension of the penalty Hamiltonian we introduced above.

4.2.1 Logical AND-gadget

We will now show the use of the penalty Hamiltonian constructed in equation 7. We make the simulator Hamiltonian:

$$H_{\text{sim}} = N_m N_3 + H_{\text{AND}}$$

For $\Delta \geq 1$, this Hamiltonian has the property that its low-energy subspace is characterized by $\mathcal{H}_{\leq \Delta} = \text{span}\{|n_1 n_2 n_3 n_m\rangle | n_m = n_1 \wedge n_2\}$ or $n_m = n_1 \cdot n_2$ when viewed as binary numbers instead of literals. Thus the term $N_m N_3$ has the same action as $N_1 N_2 N_3$ on this space in the sense that $N_m N_3 |\psi\rangle = N_1 N_2 N_3 |\psi\rangle$ for all $|\psi\rangle \in \mathcal{H}_-$ because $n_m = n_1 n_2$. So via the Logical gadget, we have a 2-local interaction that simulates a 3-local one perfectly as long as we're in the low-energy subspace of the simulator. Notice also that if $N_1 = N_1^z, N_2 = N_2^z, N_3 = N_3^x$ the action of H_{sim} is the same as H_{Toff} on qubits 1, 2 and 3.

Thus, it seems like we have simulated the Toffoli gate with only 2-local interactions. Here it depends on what one means: If we know that we start out in the low-energy subspace then we have simulated a Toffoli perfectly. If instead, we think about the process operationally, we run into an issue. Imagine that we, as an example, start in the state $|\psi\rangle = \frac{1}{\sqrt{2}} |0_1 0_2 0_3 0_m\rangle + \frac{1}{\sqrt{2}} |1_1 1_2 0_3 0_m\rangle$ and want to apply a Toffoli controlled on qubits 1 and 2 and with target qubit 3. The promise of being in the low-energy subspace feels the most natural if it worked in parallel, that is:

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|0_1 0_2 0_3 0_m\rangle + |1_1 1_2 0_3 0_m\rangle) \xrightarrow[\text{Low-energy}]{\text{Promise}} |\varphi\rangle = \frac{1}{\sqrt{2}} (|0_1 0_2 0_3 0_m\rangle + |1_1 1_2 0_3 1_m\rangle)$$

Which would mean that the simulated gate becomes:

$$|\Psi\rangle = \exp(-i\pi H_{\text{sim}}) |\varphi\rangle = C_m X_3 |\varphi\rangle = C_1 C_2 X_3 |\varphi\rangle = \frac{1}{\sqrt{2}} (|0_1 0_2 0_3 0_m\rangle + |1_1 1_2 1_3 1_m\rangle)$$

Which looks like what we wanted, but the system has clearly been entangled with the ancilla qubit. Quantitatively, when tracing out the ancilla;

$$\rho = \text{Tr}_m[|\Psi\rangle\langle\Psi|] = \frac{1}{2} |0_1 0_2 0_3\rangle\langle 0_1 0_2 0_3| + \frac{1}{2} |1_1 1_2 1_3\rangle\langle 1_1 1_2 1_3|$$

we produce what is a totally mixed state. Thus, in order to finish the gadget in respect to applying gates, one must somehow decouple the ancilla qubit from the rest of the system. One could do this by modifying the Hamiltonian such that its low-energy-subspace corresponds to some fixed logical state of the ancilla (either $|0\rangle_m$ or $|1\rangle_m$) or by applying the proper operator conditioned on the rest of the system such that it ends up decoupled; here a Toffoli would be necessary to apply to the ancilla bit controlled on bits 1 and 2. This was exactly the gate we originally intended to simulate, so this modification would make the gadget unfeasible. We talk more on this in section 5.2.

In the following section, we will introduce the novel "Logical chain gadget" that we constructed to overcome connectivity issues on an interaction graph.

4.2.2 Chain Gadget

The strength of the Logical gadget is obvious, and the application of the Logical AND-gadget seems like a natural usage of the framework. One of the downsides of the above construction is that you need a setup for which qubit 1,2 and m can interact with full connectivity. The limitations of the connectivity graphs in a system will in general be a bottle-neck for which operations are possible on a quantum computer. We will now introduce the novel chain gadget construction which can aid in such a connectivity shortage by propagating information on through a graph.

The chain gadget consists of a Hamiltonian that is a sum of link penalty terms that corresponds to creating a chain of equal logical variables. One link of the chain is build up of a penalty Hamiltonian of the form:

$$H_{\text{link},1\leftrightarrow 2} = \Delta(N_1 - N_2)^2 = \Delta(N_1 + N_2 - 2N_1 N_2)$$

Where the expansion of the paranthesis comes from the fact that each N_i is a projector and that $[N_1, N_2] = 0$. The low-energy-subspace of this Hamiltonian exactly corresponds to the logical statement “ $N_1 = N_2$ ”. Therefore, by summing these links from index 1 to K :

$$H_{\text{chain}, 1 \leftrightarrow K} = \sum_{k=1}^{K-1} H_{\text{link}, k \leftrightarrow k+1}$$

We form a chain of qubits, whose low-energy subspace exactly becomes the states for which “ $N_1 = \dots = N_k$ ”. Thus, if we start out in the initial state $|\psi_i\rangle = |\varphi_1\rangle |0_2 \dots 0_N\rangle$, we will, if the low-energy promise can be implemented in the right way, go to the final state $|\psi_f\rangle = |\varphi_1\rangle |\varphi_2\rangle \dots |\varphi_N\rangle$. In that sense we can propagate information through the interaction graph via the gadget, where we use every qubit on the way as a resource.

One can merge the Logical-AND and the Logical chain to make the Logical-AND work over arbitrarily long distances on a graph. Imagine a system where qubits 1 and 2 share neighbour qubit m_1 and we have a path from this qubit to qubit 3 through qubits m_2, m_3, \dots, m_k . Then we can construct the Hamiltonian:

$$H_{\text{sim}} = N_{m_k} N_3 + H_{\text{AND}} + H_{\text{chain}, m_1 \leftrightarrow m_k}$$

Where the AND-Hamiltonian acts on qubits 1, 2 and m_1 . The two last terms act as penalty Hamiltonians and exactly force the low-energy subspace to be characterized by:

$$\mathcal{H}_{\leq \Delta} = \text{span}(|n_1 n_2 n_{m_1} \dots n_{m_k} n_3\rangle |n_{m_1} = n_1 \wedge n_2, \quad n_{m_1} = n_{m_2} = \dots = n_{m_k})$$

and thus, by choosing $N_j = N_j^z$ for $j \in \{1, 2, m_1, \dots, m_k\}$, and $N_3 = N_3^x$, in practice we produce a CNOT with control qubit m_k and target qubit 3, where each qubit m_1 to m_k has the same logical expression and where qubit m_1 has same logical value as qubit 1 AND qubit 2. Like above, this seems like it does the trick: By applying a CNOT onto the target qubit controlled on qubit m_k , this effectively becomes a Toffoli controlled on qubits 1 and 2 and targeted on qubit 3. Thus, in this subspace, we can simulate the Toffoli interaction via a two-local interaction on any connectivity graphs.

But just like before, this produces entanglement between the target qubits and each of the ancillas, so in order to procure the Toffoli and nothing else, one would need to decouple all the ancillas. Methods for this will be proposed in section 5.2.

In the following section, we will introduce the novel Logical swap-gadget that also solves problems of limited connectivity graphs.

4.2.3 Logical Swap

An alternative way to solve the limitations of a connectivity graph comes from applying successive SWAP-operation on your qubits. The SWAP-operator is a gate on two qubits that is

characterized by interchanging the two indexes of your state, that is:

$$\begin{aligned} U_{\text{SWAP}} |00\rangle &= |00\rangle & U_{\text{SWAP}} |01\rangle &= |10\rangle \\ U_{\text{SWAP}} |10\rangle &= |01\rangle & U_{\text{SWAP}} |11\rangle &= |11\rangle \end{aligned}$$

Intuitively, what it does is swap the location of the qubits that it's acting on. Thus, the SWAP-operator can also be used to propagate information through a graph by using it to “move” a qubit down a line.

The Logical gadget finds its strongest usages in operators that are naturally formulated to have two distinct eigenvalues, since they up to energy scaling and energy shift can become a projection. A prime example of this is exactly the SWAP-Hamiltonian, whose time-evolution generates a SWAP-gate up to a global phase after $t = \frac{\pi}{4}$ time:

$$H_{\text{SWAP},1\leftrightarrow 2} = \vec{\sigma}_1 \cdot \vec{\sigma}_2 = X_1 X_2 + Y_1 Y_2 + Z_1 Z_2$$

This is a well-known operator from basic Quantum Mechanics: It divides the Hilbert-space into the singlet and the triplet states, with the triplet states having an eigenvalue of 1 and the singlet state having an eigenvalue of -3 . By shifting the energy levels $H \rightarrow H - \mathbb{1}$ and scaling them $H \rightarrow -\frac{1}{4}$, we get that the SWAP-Hamiltonian is physically equivalent to the projection:

$$H_{\text{SWAP}} \simeq |\psi_{-}\rangle \langle \psi_{-}|$$

Where $|\psi_{-}\rangle$ is the singlet state given by:

$$|\psi_{-}\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)$$

So the SWAP-Hamiltonian is physically equivalent to a projection, which makes it a prime candidate for the Logical gadget construction. Sadly, the projection is not a tensor product of 1-local projections, so one needs to transform the state to a product state in order for the Logical gadget to be applicable.

Luckily, the preparation of such a Bell-State via two-local gates is well-established in the literature. One can make the Bell-state via:

$$|\psi_{-}\rangle = C_1 \text{NOT}_2 \cdot H_1 |11\rangle$$

Where $C_1 \text{NOT}_2$ is a NOT-operation controlled on the first qubit applied to the second and H_1 is a Hadamard gate applied to the first qubit. As such, we see from the above that the interaction can be written as:

$$H_{\text{SWAP}} \simeq |\psi_{-}\rangle \langle \psi_{-}| = C_1 \text{NOT}_2 \cdot H_1 |11\rangle \langle 11| H_1 C_1 \text{NOT}_2$$

And applied as a gate, we get that:

$$U_{\text{SWAP}} = (e^{i\frac{\pi}{4}}) \exp\left(-i\frac{\pi}{4} H_{\text{SWAP}}\right) = \exp(i\pi |\psi_{-}\rangle \langle \psi_{-}|) = C_1 \text{NOT}_2 \cdot H_1 \exp(i\pi |11\rangle \langle 11|) H_1 C_1 \text{NOT}_2$$

We have that $|11\rangle\langle 11| = N_1^z \otimes N_2^z$ and thus the Logical Gadget becomes easily applicable. For instance, if qubit 1 and 2 are separated by a chain of qubits m_1, \dots, m_k we can apply a chain gadget from qubit 1 to m_k and add an interaction between qubits m_k and 2:

$$H_{\text{sim,Project}} = N_{m_k}^z N_2^z + H_{\text{chain},1 \leftrightarrow m_k}$$

Under the promise of being in the low-energy-subspace, this will exactly simulate the wanted action H_{SWAP} between qubit 1 and 2. Luckily, also the CNOT's are easily synthesizable through Logical gadgets since:

$$\exp(-i\pi N_1^z N_2^x) = C_1 \text{NOT}_2$$

And thus, we can simulate a CNOT between qubit 1 and 2 by another chain:

$$H_{\text{sim,CNOT}} = N_{m_k}^z N_2^x + H_{\text{chain},1 \leftrightarrow m_k}$$

In the end, the SWAP-gate can be simulated by three successive Logical gadgets with Hadamards in between them. Through this protocol, one would have swapped around the states of qubit 1 and 2, but coupled everything to the rest of the ancillas as well. These ancilla would need to be decoupled from the system in order to continue any quantum calculation.

This simulation of the SWAP-gate seems to succeed in our framework, but one needs three successive usages of Logical gadgets in order to do so. Operationally, our discussions seem to imply that the promise of being in the low-energy-subspace is either computationally expensive or only approximately true, see section 5.2 for details. Thus, the need to apply several gadgets to a gate-model seems unfeasible or as though it doesn't save the hardware-wise complexity of implementation.

Today, the SWAP-gate is used to overcome the limitations of connectivity on physical quantum hardware: Its action is to interchange the states of two neighbouring qubits, whilst respecting entanglement and superposition. By applying it in succession, one can make qubits that are far apart on the connectivity graph come together such that one can apply gates on them. After application, one can swap the states back so that the transferred qubit finds its initial location on the graph. This means that if the shortest path between two qubits i and j is L , one needs to apply $L - 1$ SWAP gates before applying some 2-local unitary and then $L - 1$ SWAP gates again to go back to the original configuration. In conclusion this process takes $2L - 1$ 2-qubit gates. In contrast, our simulator needs three usages of gadgets and 2 applications of Hadamards to apply a long-distance SWAP-gate but utilizes and couples to every ancilla qubit between qubit i and j . Thus, the protocol in which you apply the Logical SWAP-gadget, apply your 2-local unitary and use the SWAP-gadget to go back would cost 6 applications of gadgets, 4 Hadamards and the need to decouple every ancilla. At this level, whether the gadget saves implementation complexity or not boils down to whether the low-energy promise is easily implementable and whether a decoupling mechanism can be achieved.

4.2.4 Combinations of Logical Gadgets

The logical gadgets we have so far constructed all consist of a penalty Hamiltonian that enables two-local interactions to behave like they were of higher locality but we have yet to examine the application of multiple of these penalty Hamiltonians at the same time. There are two natural ways to combine gadgets: In parallel or in series, and we'll define what we mean by both of these terms in the following paragraph.

Putting penalty terms in series would be to apply a sum of penalty terms like the following:

$$H_{\text{series}} = \Delta_1(3N_{m_1} - 2N_1N_{m_1} - 2N_2N_{m_1} + N_1N_2) + \Delta_2(3N_{m_2} - 2N_3N_{m_2} - 2N_{m_1}N_{m_2} + N_3N_{m_1})$$

This Hamiltonian has a low-energy subspace characterized by the statement “ $(N_{m_2} = N_{m_1} \wedge N_3)$ ” and “ $(N_{m_1} = N_1 \wedge N_2)$ ”, which combined implies that “ $N_{m_2} = N_1 \wedge N_2 \wedge N_3$ ”. This means that the interaction term $H_{\text{int}} = N_4N_{m_2}$ would act like the 4-local interaction $N_1N_2N_3N_4$ in the low-energy subspace.

One could instead add the Logical gadgets together in the following way:

$$H_{\text{parallel}} = \Delta_1(3N_{m_1} - 2N_1N_{m_1} - 2N_2N_{m_1} + N_1N_2) + \Delta_2(3N_{m_2} - 2N_3N_{m_2} - 2N_4N_{m_2} + N_3N_4) \\ + \Delta_3(3N_{m_3} - 2N_{m_1}N_{m_3} - 2N_{m_2}N_{m_3} + N_{m_1}N_{m_2})$$

This Hamiltonian has a low-energy-subspace characterized by the statement “ $(N_{m_1} = N_1 \wedge N_2)$ ”, “ $(N_{m_2} = N_3 \wedge N_4)$ ” and “ $(N_{m_3} = N_{m_1} \wedge N_{m_2})$ ”, which together implies the property that “ $N_{m_3} = N_1 \wedge N_2 \wedge N_3 \wedge N_4$ ”. We denote this process by putting Logical gadgets in ”parallel”. In other words, the only difference between putting Logical gadgets in parallel or in series comes from whether the gadgets first acts on target qubits and then mediates information through ancillas or that the gadgetization happens successively on target and ancilla qubits.

Notice that the penalties Δ_1 , Δ_2 and Δ_3 don't have a natural order in either the serialization or parallelization of Logical gadgets. The construction works as long as they are larger than 1 but one could distinguish between them in order to get different penalties from breaking one of the logical statements instead of another.

One could continue to do this successively, either putting the Logical gadget in series or parallel to get a target Hamiltonian of arbitrarily complex locality, see figure 9 for a schematic.

Magically, we find that there are no demands on how the gap parameters Δ_i should scale; as long as we are in the low-energy subspace, they simulate the wanted interaction perfectly on the target qubits. Less magically, we see from figure 9 that the needed amount of ancilla qubits scale linearly with the locality of the target Hamiltonian both when putting the gadgets in parallel and in series.

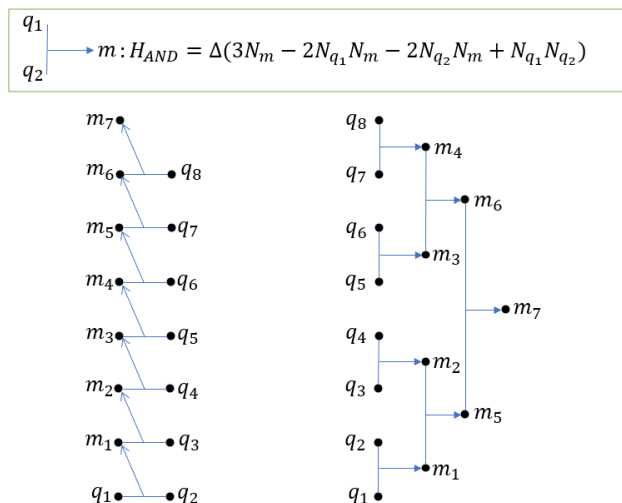


Figure 9: Schematic for how one could put Logical gadgets either in series (left) or in parallel (right). The m 's stand for ancilla qubits where q 's stand for target qubits. In both cases, the low-energy subspace has the property that “ $N_{m_7} = \bigwedge_{i=1}^8 N_{q_i}$ ” and thus $H_{\text{int}} = N_{m_7}N_{q_9}$ acts as a 9-local operator. Notice that the two constructions have the same amount of operators and ancilla qubits.

4.3 Magnus Gadgets

Our construction so far have shown many usecases, but they are alike in the sense that they work with simulator Hamiltonians that are time-independent. We will now introduce our novel Magnus gadget, which uses time-dependent simulator Hamiltonians. To start with, we will talk about the concept of a Catalyst gadget, an idea inspired by the work of [17]. We will then go on to introduce the framework and two applications of the Magnus gadget.

One of the first ideas of a catalyst Hamiltonian construction was introduced in [17]. Here they proved within the framework of local quantum operations and classical communication (LQCC), that by adding an ancilla qubit it is possible to apply channels on your target qubits that weren't without the existence of the ancilla. It is with this in mind that we are inspired to introduce the concept of a time-dependent Catalyst gadget.

Such a gadget would attempt something entirely different than the Perturbative and Logical gadget: By adding an ancilla qubit, it would attempt to simulate a target time-evolution with a time-dependent simulator Hamiltonian that is the sum of a set of Hamiltonians. That is:

$$H(t) = \sum_{k=1}^n u_k(t)H_k$$

Where $u_k(t)$ is the pulse strength of each Hamiltonian as a function of time and the H_k 's can be drawn from some fixed set of interactions. The inspiration behind this construction is that the introduction of a sum of time-dependent interactions might give non-trivial time evolutions. For this to actually produce exciting dynamics, the set of Hamiltonians definitely have to be non-commutative with respect to each other. Furthermore, we will introduce an ancilla qubit, which might in general help the time-evolution go towards the target unitary. The ancilla would then hopefully work as a catalyst to procure a given Hamiltonian and thus induce interactions that would be impossible without it but without the ancilla qubit being consumed in the process. Thus, this gadget would be a gadget-like-pendent to the concept of a catalyst in chemistry. Mathematically, we hope to apply pulses such that the generated time-evolution U_{sim} has the property that for any state of the form $\rho_{\text{tot}} = \rho \otimes |0\rangle\langle 0|_m$, we get that:

$$\|U_{\text{target}}\rho U_{\text{target}} - \text{Tr}_m(U_{\text{sim}}\rho_{\text{tot}}U_{\text{sim}})\|_1 \leq \varepsilon$$

Such that tracing out the ancilla system, we get the wanted time-evolution to some error $\varepsilon > 0$. This is one of the most general problems in all of quantum mechanics: To solve the Schrödinger equation with a time-dependent Hamiltonian that doesn't commute with itself at different times. A solution to this problem is formally known as the Dyson series. The goal of the perturbative formulation of quantum field theory and condensed matter theory is to approximate this dynamics to some order in the Dyson series and both disciplines do so via the methods of Feynman diagrams.

We will in the following section introduce an example of a catalyst gadget, which we name a Magnus gadget. It works via another formal solution to the Schrödinger equation called the Magnus expansion, which is qualitatively rather different than the Dyson series.

4.3.1 Magnus expansion

The Schrödinger equation for the time-evolution operator with a time dependent Hamiltonian takes the form:

$$\dot{U}(t) = -iH(t)U(t)$$

For which the formal solution typically used in physics is the Dyson series:

$$U(t) = \mathcal{T} \exp\left(-i \int_0^t H(t')dt'\right)$$

Where the exponential should be understood as its power series and \mathcal{T} is the time-ordering operator that acts on each term in the power series such that you always multiply earlier times to the right in the product. One would typically expand this perturbatively, truncate the series to some order and then do the integrals as Feynmann Diagrams.

Another method of solving this formally is via the Magnus expansion, which is what we'll use in the following section. The Magnus expansion takes the form:

$$U(t) = \exp(\Omega(t))$$

Where $\Omega(t)$ itself has an expansion of the form [5]:

$$\Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t)$$

With the first three terms given by:

$$\begin{aligned} \Omega_1(t) &= -i \int_0^t H(t_1) dt_1 \\ \Omega_2(t) &= -\frac{1}{2} \int_0^t \int_0^{t_1} [H(t_1), H(t_2)] dt_2 dt_1 \\ \Omega_3(t) &= \frac{i}{6} \int_0^t \int_0^{t_1} \int_0^{t_2} [H(t_1), [H(t_2), H(t_3)]] + [H(t_3), [H(t_2), H(t_1)]] dt_3 dt_2 dt_1 \end{aligned}$$

Each term in the expansion of $\Omega(t)$ gets intrinsically more complex but is defined via recursive applications of commutators and sums of such commutators integrated from earlier to later times. Notice that $\Omega_1(t)$ is the well-known solution to the Schrödinger equation when the Hamiltonian commutes with itself at different times. All the extra terms come as corrections to this naive guess on the solution.

The Magnus expansion looks a lot like the Dysons series but it does have some advantages. A truncation of $\Omega(t)$ to any order will still leave the truncated time-evolution $U_n(t) = \exp(\sum_{k=1}^n \Omega_k(t))$ unitary. Thus, by interpreting the object $\Omega(t)$ as an effective Hamiltonian, it is obvious that we can use this expansion as a means to simulate the time evolutions of more complex Hamiltonians. This method is very similar to the one used when looking at Floquet Hamiltonians, and they become identical if $H(t)$ is periodic and one evaluates the time-evolution stroboscopically.

Another feature of this method is that the Magnus expansion comes in the language of commutators instead of the language of products and time-orderings native to the Dyson series, which sometimes is easier to deal with. In our examples that sure is the case.

One of the key features of the Magnus expansion that makes it difficult to use in most quantum physics is its criteria for convergence. One of the strongest proven sufficient conditions for the convergence of the Magnus expansion at time T is that the following bound on the Hamiltonian is upheld [7]:

$$\int_0^T \|H(t)\| dt < \pi$$

There exists examples for which the Magnus expansion both does and doesn't converge where the integral above is larger than π . During the constructions in this thesis, the above condition

will in general not be upheld but, as is the way of true physicists, we will still assume that the Magnus expansion converges. Thus, by not being able to prove whether the Magnus expansion actually works, the framework of the Magnus gadget is more of a heuristical method for finding interesting time-dependent Hamiltonians than a rigorous mathematical methodology. We will in the following section introduce our first construction of the Magnus gadget.

4.3.2 CNOT Construction

We will now use the Magnus expansion to simulate a CNOT-target Hamiltonian between bits 1 and 2 from a simulator Hamiltonian of the form:

$$H(t) = u^x(t)N_1X_m + u^z(t)N_2Z_m$$

For some projections N_1, N_2 and pulses $u^x(t), u^z(t)$ for which $\frac{u^x(t)}{u^z(t)}$ isn't a constant for the entire interval. The last requirement ensures that the Hamiltonian doesn't commute with itself at different times and thus produces non-trivial dynamics. This Hamiltonian will be activated on an interval, for our case the interval $t \in [0, T]$.

We will furthermore construct our activation pulses such that:

$$\int_0^T u^x(t)dt = \int_0^T u^z(t)dt = 0$$

$$u^x(t) = u^x(T - t), \quad u^z(t) = u^z(T - t)$$

The first requirement is there to make sure that the first order term "integrates out" $\Omega_1(T) = 0$. The second requirement gives time-reversal symmetry around the middle of the process, and is a sufficient condition to force even terms in the expansion to be eliminated $\Omega_{2k}(T) = 0$ [8].

By the above construction the leading order term of the Magnus expansion is the third order term. By explicitly inserting our Hamiltonian into the formula above we get:

$$\begin{aligned} \Omega_3(t) &= -\frac{i}{6}N_1N_2X_m \int_0^t \int_0^{t_1} \int_0^{t_2} u^x(t_1)u^z(t_2)u^z(t_3) + u^z(t_1)u^x(t_2)u^z(t_3) - 2u^z(t_1)u^x(t_2)u^z(t_3)dt_3dt_2dt_1 \\ &\quad -\frac{i}{6}N_1N_2Z_m \int_0^t \int_0^{t_1} \int_0^{t_2} u^z(t_1)u^x(t_2)u^x(t_3) + u^x(t_1)u^x(t_2)u^z(t_3) - 2u^x(t_1)u^z(t_2)u^x(t_3)dt_3dt_2dt_1 \\ &\equiv -iN_1N_2(u_3^x(t)X_m + u_3^z(t)Z_m) \end{aligned}$$

Where we define $u_3^x(t)$ and $u_3^z(t)$ as the integrals of the previous lines such that the equation holds.

The next statement takes the method from being a provably true protocol for simulating target Hamiltonians under the assumption of a converging Magnus expansion to becoming an even more heuristic method: By recursively applying more commutators, every even term should hopefully become of the form $\Omega_{2k}(t) = u_{2k}^y(t)N_1N_2Y_m$ for suitable activation pulse $u_{2k}^y(t)$. Every odd term will be sums of commutators of the even and odd terms, which again hopefully should be of the

form $\Omega_{2k+1}(t) = N_1 N_2 (u_{2k+1}^x(t) X_m + u_{2k+1}^z(t) Z_m)$ for suitable functions $u_{2k+1}^x(t)$ and $u_{2k+1}^z(t)$. This is a statement I am fairly certain can be proven but we have not been able to do so in this thesis.

The even terms integrate to 0 by the form of the activation pulses [8] and the odd terms are hopefully all of the same form as $\Omega_3(t)$ for fitting $u_{2k+1}^x(t)$ and $u_{2k+1}^z(t)$ pulses. By adding them all together, we get:

$$\Omega(T) = \sum_{k=1}^{\infty} \Omega_k(T) = -i N_1 N_2 (v^x(T) X_m + v^z(T) Z_m)$$

Where we have defined the renormalized pulses:

$$v^x(t) \equiv \sum_{k=1}^{\infty} u_{2k+1}^x(t), \quad v^z(t) \equiv \sum_{k=1}^{\infty} u_{2k+1}^z(t)$$

Thus, the Magnus expansion gives us insight to what other Hamiltonian would have produced the same time evolution. By defining the parameters $\theta(t) \equiv \sqrt{v^x(t)^2 + v^z(t)^2}$, $B^x(t) = \frac{v^x(t)}{\theta(t)}$ and $B^z(t) = \frac{v^z(t)}{\theta(t)}$, we can rewrite $\Omega(T)$ as:

$$\Omega(T) = -i \theta(T) N_1 N_2 (B^x(T) X_m + B^z(T) Z_m)$$

We can see from this expression that we can interpret the time-evolution as the same one that comes from the time-independent Hamiltonian:

$$H_{\text{target}} = N_1 N_2 (B^x(T) X_m + B^z(T) Z_m)$$

After waiting $\theta(T)$ time. From this formulation, it becomes clear that we can interpret the parameters $\theta(t)$ as a renormalized time-parameter and $B^x(t)$ and $B^z(t)$ as normalized activation pulses on the ancilla.

We succeeded in actually characterizing the time-evolution of this system even though the Hamiltonian is time-dependent and doesn't commute with itself at different times. The method does hold its problems though. We don't actually know what is going on in the sense that the parameters $B_x(t)$, $B_z(t)$ and $\theta(t)$ are unknown to us, unless we calculate the Magnus expansion to arbitrary order. Furthermore, the method hasn't been proven in a strict mathematical sense and just works as a heuristic idea for how the solution could look like. Thus, in order to use it, we will have to numerically simulate the solution to figure out if the heuristic worked and then to characterize all these three parameters. But as soon as we've done so for some fixed ending time T and activation pulses $u^x(t)$ and $u^z(t)$, we can use the construction iteratively. That is, for any natural number $n \in \mathbb{N}$ we can get $U(nT)$ by applying the Hamiltonian successively: $U(nT) = U(T)^n$, by the semi-group property of the time-evolution.

A method typically used in quantum computing to get a time-evolution at later times more

rapidly is to crank up the energies, which here means to crank up the amplitudes of our activation pulses. Unfortunately, this doesn't work here, since the renormalized pulses $v^x(t)$ and $v^z(t)$ aren't linear in the amplitude of the starting pulses; they are defined as the sum of some iterative process of integrating differences of products of activation pulses from earlier times to later times. In the end, in order to learn about the non-linear behaviour of $\theta(t)$ as a function of pulse-amplitudes, one would definitely need to either calculate these numerically or approximate them as a truncation of the Magnus expansion.

Once we know the three parameters that characterize the target Hamiltonian at time T , we can finally figure out which unitary operations we have simulated. We can write the time evolution as:

$$\begin{aligned} U(T) &= \exp(\Omega(T)) = \exp(-i\theta(T)N_1N_2(B^x(T)X_m + B^z(T)Z_m)) \\ &= (\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes V_B) \exp(-i\theta(T)N_1N_2Z_m) (\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes V_B^\dagger) \end{aligned}$$

Where the unitary V_B is the matrix that diagonalizes the action on the ancilla qubit m . In particular, it is the $SU(2)$ -matrix that represents rotation around the Y -axis in real space with angle $\varphi = \arctan\left(\frac{B_x}{B_z}\right)$:

$$V_B = \begin{pmatrix} \cos(2\varphi) & \sin(2\varphi) \\ -\sin(2\varphi) & \cos(2\varphi) \end{pmatrix} \quad (8)$$

One would get rid of this by making the relevant $SU(2)$ -rotation before applying any time-dependent pulse-driven Hamiltonian.

From the above, there are two obvious, relevant time-evolutions we can get out of the construction: A CNOT and a control-control-unitary. The first is built by choosing $N_1 = N_1^z$, $N_2 = N_2^x$ and by applying the Hamiltonian for enough time or over enough iterations to get $\theta(T) = \pi$. Then we get:

$$\begin{aligned} U(T) &= \exp(-i\pi N_1^z N_2^x (B^x(T)X_3 + B^z(T)Z_3)) = \sum_{n=0}^{\infty} \frac{(-i\pi N_1^z N_2^x (B^x(T)X_3 + B^z(T)Z_3))^n}{n!} \\ &= \mathbb{1} + (\cos(\pi) - 1) N_1^z N_2^x - i \sin(\pi) N_1^z N_2^x (B^x(T)X_m + B^z(T)Z_m) = C_1 \text{NOT}_2 \end{aligned}$$

The control-control-unitary comes from choosing $N_1 = N_1^z$, $N_2 = N_2^z$ and have renormalized time $\theta(T) = \pi/2$:

$$\begin{aligned} U(T) &= (\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes V_B) (\mathbb{1} + (\cos(\pi/2) - 1) N_1^z N_2^z - i \sin(\pi/2) N_1^z N_2^z Z_m) (\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes V_B^\dagger) \\ &= C_1 C_2 (-i V_B^\dagger Z_m V_B) \end{aligned}$$

That is, we simulate the unitary for which if both qubits 1 and 2 are in state $|1\rangle$, we apply the operator $-i V_B^\dagger Z_m V_B$ to qubit m and else we do nothing.

Notice that these constructions are now exact and not under a promise of being in the low-energy subspace of any Hamiltonian, unlike for the Perturbative and Logical gadget. Also, notice that the first construction is what we would call a "Catalyst gadget" in the sense that it factors out the interactions on the mediator qubit and therefore we call this construction a CNOT-gadget. The other one isn't a Catalyst gadget though, since it couples all three qubits to each other. Notice also that the rigor of the arguments for why the construction works is a lot more loose than both the Perturbative and Logical gadgets in the sense that we mainly gave a heuristic argument for how $\Omega(T)$ would look to all orders. Therefore we must remember that a proof has to be made before these are formal statements. We will in section 4.3.5 show examples for which we've simulated the system numerically and figure out that our statements are actually correct. In the next section, we will continue working on these heuristics to create interactions of even higher locality.

4.3.3 Toffoli Constructions

From our first constructions, we see that we can simulate the time-evolutions of 2- or 3-local interactions rather easily. The reason they worked was because the non-trivial commutators couple terms acting on different systems. Thus, the commutators hold the same role in this construction as the V_{++} did in the Perturbative gadget in the sense that a non-trivial commutator simulated interactions that were of higher locality.

In order to make our construction more general, we should add more couplings to the X - or Z -term, like we added more terms in V_{++} . That is, we will construct a Hamiltonian of the form:

$$H(t) = (u^{x_1}(t)N_1 + u^{x_2}(t)N_2) X_m + u^z(t)N_3Z_m$$

We will also demand the following 12 third-order restrictions on our activation pulses:

$$\begin{aligned} 0 &= \int_0^T \int_0^{t_1} \int_0^{t_2} u^{x_1}(t_1)u^z(t_2)u^z(t_3)dt_3dt_2dt_1 = \int_0^T \int_0^{t_1} \int_0^{t_2} u^{x_2}(t_1)u^z(t_2)u^z(t_3)dt_3dt_2dt_1 \\ &= \int_0^T \int_0^{t_1} \int_0^{t_2} u^z(t_1)u^z(t_2)u^{x_1}(t_3)dt_3dt_2dt_1 = \int_0^T \int_0^{t_1} \int_0^{t_2} u^z(t_1)u^z(t_2)u^{x_2}(t_3)dt_3dt_2dt_1 \\ &= \int_0^T \int_0^{t_1} \int_0^{t_2} u^z(t_1)u^{x_1}(t_2)u^z(t_3)dt_3dt_2dt_1 = \int_0^T \int_0^{t_1} \int_0^{t_2} u^z(t_1)u^{x_2}(t_2)u^z(t_3)dt_3dt_2dt_1 \\ 0 &= \int_0^T \int_0^{t_1} \int_0^{t_2} u^z(t_1)u^{x_1}(t_2)u^{x_1}(t_3)dt_3dt_2dt_1 = \int_0^T \int_0^{t_1} \int_0^{t_2} u^z(t_1)u^{x_2}(t_2)u^{x_2}(t_3)dt_3dt_2dt_1 \\ &= \int_0^T \int_0^{t_1} \int_0^{t_2} u^{x_1}(t_1)u^{x_1}(t_2)u^z(t_3)dt_3dt_2dt_1 = \int_0^T \int_0^{t_1} \int_0^{t_2} u^{x_2}(t_1)u^{x_2}(t_2)u^z(t_3)dt_3dt_2dt_1 \\ &= \int_0^T \int_0^{t_1} \int_0^{t_2} u^{x_1}(t_1)u^z(t_2)u^{x_1}(t_3)dt_3dt_2dt_1 = \int_0^T \int_0^{t_1} \int_0^{t_2} u^{x_2}(t_1)u^z(t_2)u^{x_2}(t_3)dt_3dt_2dt_1 \end{aligned}$$

The first six requirements relate to how N_1 and N_2 would couple to each other without coupling to N_3 in $\Omega_3(T)$ and the next six requirements relate to how N_3 would couple with either N_1 or

N_2 but not both in $\Omega_3(T)$. By having the 12 requirements from above, all that is left to third order is the coupling of all three terms, and thus Magnus expansion to third order becomes:

$$\Omega_3(t) = -iN_1N_2N_3(u_3^x(t)X_m + u_3^z(t)Z_m)$$

With fitting activation pulses $u_3^x(t)$ and $u_3^z(t)$. Higher order terms involve the summation of additional successive commutators and hopefully this indicates that every higher order term holds the same form as the above third order one. This should lead to a total generator from the Magnus expansion of the form:

$$\Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t) = -iN_1N_2N_3(v^x(t)X_m + v^z(t)Z_m) \equiv -i\theta(t)N_1N_2N_3(B^x(t)X_m + B^z(t)Z_m)$$

Where we defined the pulses $v^x(t)$, $v^z(t)$ and the parameters $\theta(t)$, $B^x(t)$, $B^z(t)$ in the same manner as in the previous section:

$$v^x(t) = \sum_{k=1}^{\infty} u_{2k+1}^x(t), \quad v^z(t) = \sum_{k=1}^{\infty} u_{2k+1}^z(t), \quad \theta(t) = \sqrt{v^x(t)^2 + v^z(t)^2}, \quad B^x(t) = \frac{v^x(t)}{\theta(t)}, \quad B^z(t) = \frac{v^z(t)}{\theta(t)}$$

Which generates the time-evolution:

$$U(T) = \exp(-i\theta(T)N_1N_2N_3(B^x(T)X_m + B^z(T)Z_m))$$

And just like before, there are two natural choices for this time evolution operator: A Toffoli and a control-control-control-unitary. For $\theta(T) = \pi$ the evolution becomes:

$$U(T) = \mathbb{1} + (\cos(\pi) - 1)N_1N_2N_3 - i\sin(\pi)N_1N_2N_3(B^x(\pi)X_m + B^z(\pi)Z_m) = \mathbb{1} - 2N_1N_2N_3$$

Which for the choice $N_1 = N_1^z, N_2 = N_2^z, N_3 = N_3^x$ produces the Toffoli gate controlled on qubits 1 and 2 and applied to target qubit 3. Again, this produces a Catalyst gadget and thus we will call this construction a Toffoli-gadget.

Otherwise for $\theta(T) = \pi/2$, and the choice $N_1 = N_1^z, N_2 = N_2^z, N_3 = N_3^z$, the time-evolution becomes:

$$\begin{aligned} U(T) &= (\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \mathbb{1}_3 \otimes V_B) \exp\left(-\frac{\pi}{2}N_1^zN_2^zN_3^zZ_m\right) (\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \mathbb{1}_3 \otimes V_B^\dagger) \\ &= C_1C_2C_3 \left(-iV_BZ_mV_B^\dagger\right) \end{aligned}$$

Which should be understood as “if qubit 1, 2 and 3 are in state $|1\rangle$, we apply the gate $-iV_B^\dagger(T)Z_mV_B(T)$ to qubit m and otherwise we do nothing”. V_B is, just like in equation 8, the unitary needed to diagonalize $B^xX_m + B^zZ_m$. So by making some extra demands on the activation pulses, we could simulate both the time-evolution of a Hamiltonian that corresponds to a Toffoli and to a control-control-control-unitary onto an ancilla qubit.

Notice that this construction was even less rigorous than the previous one. We required 12 integrals of the pulses to be zero and even then we never proved that the Magnus generator had the

form we were searching for. To call this methodology anything more than a heuristic would not be fitting. But in the next section, we will make numerical simulations of concrete pulses, see that the constructions actually work as the heuristics predict and sweep the parameter space for $\theta(T)$.

4.3.4 Numerical Simulations

Up until now, our constructions were based on heuristic methods and was characterized by parameters we couldn't estimate. Now the question is whether these constructions are feasible. Does the heuristic method work? How rapidly does the renormalized time grow? Does there actually exist activation pulses that fulfill all of our requirements and doesn't produce a trivial simulated interaction? That is what we'll attempt to answer in this section. We will activate our pulses for a period of $T = \pi$, and we will kill both the first and second order term in the expansion by demanding that they integrate to zero and are even around their midpoint [8]. By lack of originality, we will choose pulses from one of the forms:

$$v(a, k, t) = a \cos(kt)$$

$$u(b, k, t) = \begin{cases} b \sin(kt) & 0 \leq x \leq \frac{\pi}{2} \\ -b \sin(kt) & \frac{\pi}{2} \leq x \leq \pi \end{cases}$$

The amplitudes a and b distinguish between a cosine and a sine pulse and the frequency $k \in 4\mathbb{N}$ is a multiple of 4 by the symmetry requirement of the pulse. Notice that both pulses are continuous, but only the cosine-pulse is differentiable.

What is the renormalized time as a function of the amplitude?

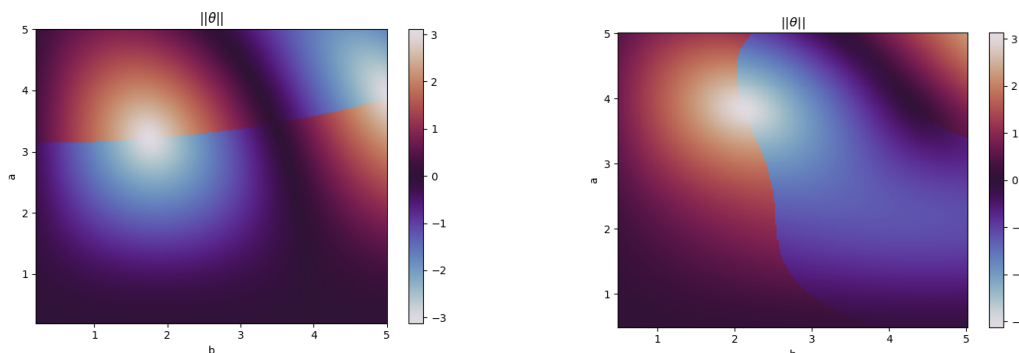
Instead of simulating a CNOT and a Toffoli, we actually simulated a control- Z and a control-control- Z -gate. We did this because it became easier to grasp whether we did it right from just observing the diagonal elements of the time evolutions. Nevertheless, these gate is equivalent to a CNOT and a Toffoli up to applications of one-local unitaries, so simulation results should remain the same.

For the CNOT construction, we used the following pulse:

$$H(t) = u(b, 4, t)N_1^z Z_m + v(a, 4, t)N_2^z X_m$$

We used the Qutip library [21] to calculate the time-evolution exactly over the period of π and find the eigenvalues of the time-evolution operator. For every simulation, we find that the time evolution operator has two distinct eigenvalues that aren't 1; a number of length unity and its complex conjugate. This is evidence that the Magnus gadget heuristic worked, since the method predicts a simulated time-evolution of the form:

$$(\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes V_B(\pi)) U(\pi) \left(\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes V_B^\dagger(\pi) \right) = C_1 C_2 P(\theta(\pi))_m$$



(a) $\theta(\pi)$ as a function of a and b for CNOT construction (b) $\theta(\pi)$ as a function of a and b for Toffoli construction

Figure 10: Simulation of $\theta(\pi)$ for the CNOT and the Toffoli construction as a function of amplitude strengths a and b . Notice that our numerical tool has by some choice given us $\theta(\pi)$ or $-\theta(\pi)$ and thus, we should understand the result under the equivalence $\theta \simeq -\theta$.

Where $P(\theta)$ is the phase gate:

$$P(\theta) = \begin{pmatrix} \exp(-i\theta) & 0 \\ 0 & \exp(i\theta) \end{pmatrix} \quad (9)$$

Thus, one can find $-\theta(\pi)$ and $\theta(\pi)$ by taking the argument of the complex eigenvalues. We do this for many different values of a and b and get the result of figure 10a.

We made the Toffoli-construction by applying the pulse:

$$H(t) = (u(b, 4, t)N_1^z + u(b, 8, t)N_2^z) Z_m + v(a, 4, t)N_3^z X_m$$

This Hamiltonian fulfills the 12 integrals requirements for the third order term that needed to be zero. Once again we find that the time-evolution operator only has 2 eigenvalues that weren't 1. This is exactly what the Magnus heuristic predicted we should, as it states that we should get a time-evolution operator of the form:

$$(\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \mathbb{1}_3 \otimes V_B(\pi)) U(\pi) (\mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \mathbb{1}_3 \otimes V_B^\dagger(\pi)) = C_1 C_2 C_3 P(\theta(\pi))_m$$

Where the phase gate $P(\theta)$ is just like before. At the same time, we found that by choosing other pulses than the one described above, we could get more than 2 eigenvalues that weren't 1 in the time evolution. Thus, this is proof that the Magnus heuristic is only a heuristic and that stronger requirements are needed to make it into a true mathematical method. But with the above choice of pulses, we do get the desired outcome.

We do the same as in the previous experiment: We simulate the time-evolution exact using the

Qutip library, find the eigenvalues and take their complex argument to get $-\theta(\pi)$ and $\theta(\pi)$. Then we plot $\theta(\pi)$ as a function of a and b . The result is shown in figure 10b.

From the plots, we see that we actually succeeded in being able to make both a Toffoli and a CNOT (where $\theta(\pi) = \pi$) from situations in which there was no direct interaction between qubits 1, 2 and 3. To answer whether the Magnus gadget is feasible becomes a question of whether the CNOT-gadget or Toffoli-gadget is faster than one would get by using 2-qubit gates in succession to construct them. For the CNOT, this consists of the following application of gates:

$$C_1NOT_2 = C_1NOT_m C_mNOT_2 C_1NOT_m$$

And for the Toffoli, this consists of the circuit diagram of fig 2, which we can write out as the following product of CNOT's and on-site gates:

$$C_1C_2NOT_3 = C_1X_2 \cdot T_2^\dagger \cdot T_1 \cdot C_1X_2 \cdot T_2 \cdot H_3 \cdot T_3 \cdot C_1X_3 \cdot T_3^\dagger \cdot C_2X_3 \cdot T_3 \cdot C_1X_3 \cdot T_3^\dagger \cdot C_2X_3 \cdot H_3$$

So the question boils down to whether the CNOT-gadget is faster than applying three CNOT's and whether the Toffoli-gadget is faster than applying 6 CNOT's and 9 on-site gates. Typically, it is the 2-qubit gates that are the most time-consuming, resource-demanding and error-sensitive, so we'll attempt to bound ourselves against these.

In order to do so, we will now define two different time-resources to compare constructions of a gate that takes time t to create: $T_{\text{weak}} \equiv \max(\text{Pulse Amplitudes}) \cdot t$ and $T_{\text{strong}} \equiv \int_0^t \|H(s)\| ds$. For both of these, we have by construction of the CNOT as a flat pulse from the Hamiltonian $H_{C_1NOT_2} = N_1^z N_2^x$ that $T_{\text{weak}} = T_{\text{strong}} = T_{\text{CNOT}} = \pi$. We introduce both of these resources because they intuitively check two different things. T_{weak} is a measure for how long it takes to create the gate regardless of parallel energy cost in the sense that if two pulses are activate at the same time, we will only care about the one with the highest amplitude. Furthermore, it counts an energy pulse as though it it a constant pulse with a strength that is the amplitude of the wave and thus favors constant pulses over cosine- or sine-pulses. T_{strong} is a measure for how much energy resource is used under the construction: If two pulses gets applied simultaneously, this measure will add their energies together in quadrature.

Since ordinary decompositions respectively require 3 and 6 CNOT's to produce, the resource the CNOT-gadget has to beat is $3T_{\text{CNOT}} = 3\pi$ and the resource the Toffoli-gadget has to beat is $6T_{\text{CNOT}} = 6\pi$ in either of these two time resources.

For the CNOT-gadget, we see from the plots that choosing b just below 2 and a just above 3, we get a phase of around π (the white dot in the middle of the plot). For this exact point, we find that $T_{\text{weak}} \approx 3\pi$ and $T_{\text{strong}} \approx 7.9$. Thus, when comparing T_{weak} the gadget doesn't introduce a time-improvement compared to the now-used decomposition but it does so provided that we compare T_{strong} .

For the Toffoli-gadget, we see that around $b \approx 2, a \approx 4$, we get a phase of π , and the time resources can be calculated to become $T_{\text{weak}} \approx 4 \cdot \pi$ and $T_{\text{strong}} \approx 10.4$. Time-wise, this introduces an improvement on the decomposition of a Toffoli both when comparing T_{weak} and T_{strong} . Thus, the Toffoli-gadget construction does give an improvement in regards to the ordinary CNOT-decomposition.

As such, we have shown that by choosing the proper sine- or cosine-pulses for your time-dependent Hamiltonian, one can make both a CNOT and a Toffoli-gate, even with no direct connectivity between the bits acted on by the gates. We found that both constructions in some way improved on ordinary decompositions into CNOT's. This is just an example though, and one could hope that this chosen pulse in no way is exhaustive in ways to simulate the Toffoli- or CNOT-interaction. There probably exist pulses that do this remarkably better than we haven't found or haven't been able to calculate the time-evolution of yet.

That there exists a pulse which simulates a Toffoli without direct connectivity is not a surprising result and could have been proven numerically by using the QuTip-library with, for instance, the GRAPE-algorithm. The difference between ordinary numerical simulations and the result we have above is that we get a closed form of our target Hamiltonian. Using QuTip would produce an approximate unitary with a pulse which may or may not be easily implementable but with no idea of which effective Hamiltonian we got from the construction.

At the same time, QuTip should generally be able to find a solution like the one we have proposed above should it exist and thus, QuTip could in practise help to find at which time-scales and at which pulse amplitudes there does exist time-dependent Hamiltonians which produce the Toffoli or the CNOT. Such numerical tools can help provide strong intuition for when it is possible and when it is not to use the Magnus gadget in concrete constructions.

5 Discussion

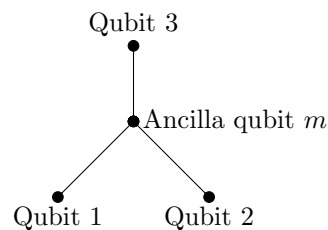
We will in this section discuss three things: Firstly, we will gather the results that we learned from the previous section and put it into the perspective of which connectivities are needed for the different constructions. Secondly, we will discuss the promise of being in the low-energy subspace of a Hamiltonian. This both consists of whether it's a realistic promise and some ideas for how one might enforce it. Lastly, we will compare the three gadgets in regards to both their strengths and weaknesses in order to give an easily accessible overview of the previous section.

5.1 Toffoli Under Different Connectivities

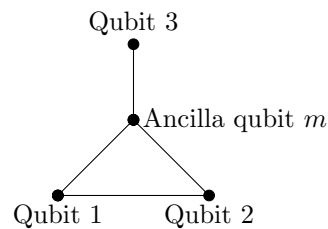
One of the major limitations of a quantum computer is its connectivity graph, which defines which qubits can be applied 2-local gates between. The sparseness of this graph defines the limitations of the computer. When working with for instance superconducting qubits, the connectivity graph is defined via which qubits have couplers between them, a property that is sown deep into the hardware and thus can't be altered after fabrication. It is with this in mind that we go on to discuss under which connectivities we can simulate the Toffoli interaction.

By the gadget construction, we succeeded in simulating the Toffoli under many different circumstances and this section serves to high-light which connectivites we have used and the error with which we can simulate these gates.

For the cross connectivity:



We saw in section 4.2 that the direct-3-local gadget could simulate a Toffoli gate with an error of $\varepsilon = O(\Delta^{-1/3})$ if one had a 3-level ancilla qudit instead of a qubit. We also saw in section 4.5 that this was the natural connectivity of the Magnus gadget, which simulated the Toffoli gate perfectly as long as we had the proper time-dependent pulses. All other constructions needed a counter term with connectivity between qubit 1 and 2 leading to the cowbell connectivity:

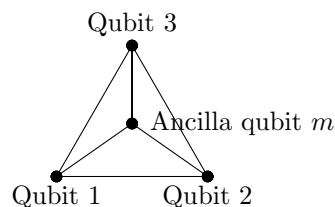


We saw in section 4.1 by the full-geometric-series-gadget that we can simulate the Toffoli Gate on this connectivity graph perturbatively with error $O(\Delta^{-1})$. This is a great deal better than what we got for the cross-connectivity, and thus, this single extra connection improves the construction to the theoretical best of the Perturbative gadget, as discussed in section 4.1.

As an even stronger result, we saw in section 4.2 that the Logical gadget can simulate the Toffoli on this connectivity up to 0 error. It is a lot better than the perturbative gadget in that sense, but it still demands to be in the low-energy subspace of a Hamiltonian. Furthermore, the Logical gadget had the issue that it induced entanglement between target and ancilla qubits which one would have to decouple before having completed the Toffoli gate.

The Magnus gadget works just as well on this graph as on the cross connectivity and might even work better with the extra connection. The problem of calculating the Magnus expansion with a term that connects qubit 1 and 2 is that the group that is closed under the actions of commutators increase drastically in size and thus, calculations become unfeasible.

For the centroid connectivity:



None of the constructions above become stronger: The Perturbative gadget and Logical gadget both work their theoretical best at the cow-bell connectivity and the Magnus gadget already works at the cross connectivity. But with this interaction graph, the Toffoli gate can be applied between any of the three qubits as control or targets and thus warrants reason to have.

5.2 Forcing qubits down into the low-energy-subspace

The gadgets considered in the literature always consist of a Hamiltonian, which has a promise of being in its low-energy subspace. This is in contrast to ordinary quantum computing where one

would want to manipulate any possible state regardless of what subspace they exist in. Therefore, from an operational point of view, the framework of gadgets requires additional work.

A way to understand why the requirement of being in a ground state is an expensive quantum resource is to look at the k -local Hamiltonian problem. If it was easily possible to transfer an arbitrary state into the ground state of any Hamiltonian, this would warrant an easy solution to this promise problem known to be QMA-complete [18]. One could even limit oneself to diagonal Hamiltonians such that the problem becomes equivalent to finding the ground state energy of a classical Ising Model and get an easy solution to a problem known to be NP-complete [9]. The method of adiabatic quantum annealing for instance does this, but there exists a bound on how fast we can reach the solution: Even the structure of the universe doesn't want us to solve NP-hard problems easily.

When it comes to condensed matter systems, it is obvious that the mathematical instrument of gadgets serves to give intuition and it is a great tool to analyze the locality complexity and dynamical properties of materials, both in regards to simulating ground-state energies but also in regard to the dynamics of the low-energy-subspace. Sadly, these real life systems typically behave so complex that only the perturbative framework can model their interactions and even then it is rather difficult to explicitly construct gadgets that simulate them. This method must in general be applied for far more complex examples than target Hamiltonians that can be written as simple product operators.

Thus, the Logical gadgets and the Pertubative gadgets work better as a simplification of quantum systems than as a recipe for approximations of quantum gates via less complex quantum gates. The question is then what gadgets can be used for in the operational context of quantum computers: Are they purely a mathematical tool or is there actually any system in which they correspond to a real life application of interactions that serve as dynamics for generating desired gates?

Below, we come up with three examples of how one could bypass the problem of operationally forcing a system to be in its low-energy subspace: Coupling the ancilla qubit to a bath, utilizing quantum annealing and creating verification protocols for the low-energy promise.

5.2.1 Couple to bath

A naive way to try to force a Hamiltonian into its low-energy subspace is to couple it to a bath of low temperature. This enables dissipation which will lead energy away from your system. The strength of this is exactly that it drives the Hamiltonian into its low energy subspace. The weakness is that typically the unique stable point is the Gibbs state [25]. Thus, if we couple the entire system to an external bath and let it cool, the ending state is not a pure state but a mixed one, independent of our starting state. Thus, globally coupling a system to its environment will mean that we lose any information about which state we started in.

If one wants to do this non-trivially, one can partially couple a system to a bath. In this framework it makes sense to couple the ancilla mediator to a bath such that it (and only it) will flip its logical state dependent on the rest of the system.

Imagine the following Lindbladian equation of motion of a dissipative system that follows a dephasing model coupled only to the ancilla mediator [11]:

$$\dot{\rho} = \mathcal{L}(\rho) = i[\rho, H] + \sum_{\omega} \gamma(\omega) \left(A(\omega)\rho A^{\dagger}(\omega) - \frac{1}{2}\{A(\omega)^{\dagger}A(\omega), \rho\} \right)$$

Where $\gamma(\omega)$ is the rates of going between two states of energy difference ω and the jumping operators $A(\omega)$ are:

$$A(\omega) = \sum_{E_2 - E_1 = \omega} P_{E_2} X_m P_{E_1}$$

Where P_{E_i} is the projection onto the subspace of energy E_i . For the jump operator and transition rates, we have that $A(-\omega) = A(\omega)^{\dagger}$ and $\gamma(-\omega) = \exp(-\beta\omega)\gamma(\omega)$ [25]. For the Logical AND-Gadget $H = H_{\text{sim}}$, the differential equation couples entries of the density matrix that corresponds to high- and low-energy states. That is for states a, b in the low-energy space and corresponding states a', b' in the high-energy space (same states but with the ancilla qubit flipped) the differential equation takes the form for relevant positive coefficients c_{ij} :

$$\begin{aligned} \dot{\rho}_{aa} &= c_{a'a'}\rho_{a'a'} - c_{aa}\rho_{aa} \\ \dot{\rho}_{a'a'} &= c_{aa}\rho_{aa} - c_{a'a'}\rho_{a'a'} \\ \dot{\rho}_{ab} &= c_{a'b'}\rho_{a'b'} - c_{ab}\rho_{ab} \\ \dot{\rho}_{a'b'} &= c_{ab}\rho_{ab} - c_{a'b'}\rho_{a'b'} \end{aligned}$$

These four differential equations produce a dynamic that flows towards a fixed point that is a modified Gibbs-state. Its final diagonal elements will have the form:

$$\begin{aligned} \rho_{aa}(\infty) &= (1 - \exp(-\beta\Delta))\rho_{aa}(0) + \exp(-\beta\Delta)\rho_{a'a'}(0) \\ \rho_{a'a'}(\infty) &= \exp(-\beta\Delta)\rho_{a'a'}(0) \end{aligned}$$

Exactly like a Gibbs state. The difference is here that the off-diagonal low-energy-low-energy and high-energy-high-energy matrix elements share the same form:

$$\begin{aligned} \rho_{ab}(\infty) &= (1 - \exp(-\beta\Delta))\rho_{ab}(0) + \exp(-\beta\Delta)\rho_{a'b'}(0) \\ \rho_{a'b'}(\infty) &= \exp(-\beta\Delta)\rho_{a'b'}(0) \end{aligned}$$

If we choose the exponent to be large $\beta\Delta \gg 1$, the model approximately preserves the low-energy states and pushes high-energy diagonal states into corresponding low-energy states. Furthermore, it even preserves correlations after this transfer in the sense that the high-energy off-diagonal

entries go to the corresponding off-diagonal low-energy entries.

Where the model fails is for the equations of motion for the off-diagonal elements that link high- to low-energy states:

$$\dot{\rho}_{aa'} = -c_{aa'}\rho_{aa'}$$

Which obviously evolves towards the fixed point:

$$\rho_{aa'}(\infty) = 0$$

Thus, correlations between high- and low-energy parts of the state will get lost. This means that the decoupling model will approximately preserve any state that solely has support on the low-energy subspace of H and approximately transfer states that solely has support on the high-energy subspace into their corresponding low-energy state. What it can't do is preserve the coherence of a state that has support on both.

So the above construction almost works for the Logical gadget. The sad part is that it fails at what we hoped to succeed at: Preserve the low-energy part of the wave-function and simultaneously move any high-energy part into its corresponding low-energy part. So the only example for which the above model solves our problem, is when we're already in the low-energy subspace or when we're only in the high energy subspace. Then we approximately end up with a state for which the Logical gadget will have worked perfectly.

5.2.2 Annealing

The method of quantum annealing is used widely in the context of quantum complexity as an alternative to the typical universal gate model used in quantum computing. The two models have been proven to be equivalent in theory since they can simulate the other effectively [20], but on existing hardware, only simulating annealing through universal gate computers is feasible. Still, this different way of thinking about quantum problems has many strengths since most tasks in reality can be naturally formulated as the minimization of some cost-function. The only question of whether this is then feasible or implementable on real quantum hardware comes as the question "can we physically implement a Hamiltonian that represents this cost function?".

The method of quantum annealing stems from the adiabatic theorem. The adiabatic theorem concerns the problem of the time-dependent Schrödinger equation with a time-dependent Hamiltonian:

$$i\frac{\partial\psi_\tau(s)}{\partial s} = \tau H(s)\psi_\tau(s)$$

Where the variable $s = t/\tau$ represents a rescaled time and is typically put to be between $s \in [0, 1]$. τ then represents how long a process takes to go from Hamiltonian $H(0)$ to $H(1)$. To solve this

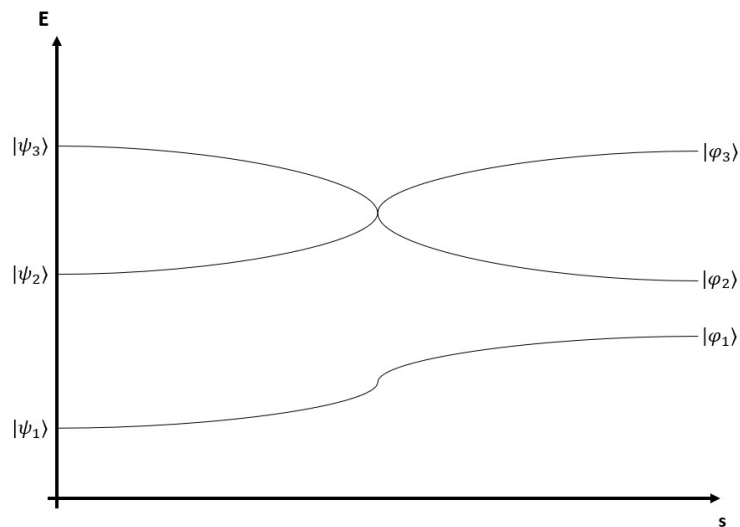


Figure 11: Graphical representation of an annealing process: How will the eigenstates evolve as a function of time? The adiabatic theorem states something very strong about the evolution of states if there is a gap. There also exists an adiabatic theorem without a gap, that demands analyticity of the spectral projections in a way that is difficult to ensure.

equation is one of the most general problems of non-relativistic quantum mechanics, but the adiabatic theorem states something rather strong about the behaviour of each eigenstate. The most general version of it was introduced in [2] when there is a gap in the energies of the eigenstates for all times:

Theorem 2. *Suppose that $P(s)$ is a smooth finite rank spectral projection, for the bounded, smooth Hamiltonian $H(s)$. Then, the evolution of the initial state $\psi_\tau(0) \in \text{Range}(P(0))$, is such that $\text{dist}(\psi_\tau(s), \text{Range}(P(s))) \leq o(1)$, where the upper bound should be seen as a decreasing function of τ that goes to 0 for $\tau \rightarrow \infty$.*

The adiabatic theorem can be formulated uniformly as the following: If you start in the ground state of $H(0)$, you end in the ground state of $H(1)$ as long as the change from $H(0)$ to $H(1)$ happens slowly enough. For a graphical representation, see figure 11.

It seems that annealing is a natural language to use when it comes to forcing a state into the low-energy subspace of a fixed Hamiltonian. When it comes to adiabatic dynamics of the ground state in practise, there exists the natural bound that τ should grow like the reciprocal of the energy-gap between the first and the second energy level. If there are energy crossings, this bound doesn't work but Theorem 2 is still true under the assumption that your spectral projection $P(s)$ has the analytical property that $\lim_{s' \rightarrow s^-} P(s') = \lim_{s' \rightarrow s^+} P(s')$ for every $s \in [0, 1]$ [2]. A first guess for

an annealing-process is the annealing Hamiltonian that linearly interpolates between something controllable and our simulator Hamiltonian:

$$H_{\text{anneal}}(s) = H_0(1 - s) + sH_{\text{sim}}$$

Where H_0 is some start-Hamiltonian such that the annealing process works as effective as possible. In the example of the Logical AND-gadget, one would want to start out in the state $|\psi\rangle = |\varphi\rangle_{1,2,3} |0\rangle_m$, that is in some state on qubits 1,2 and 3 but with the knowledge of the ancilla being in the $|0\rangle_m$ state. Thus if we choose to apply a starting Hamiltonian of the form $H_0 = -\Delta Z_m$, the ancilla qubit will start in its ground state. Should this annealing process be successful, we would start in the low-energy subspace of H_0 and end up in the low-energy subspace of the simulator Hamiltonian.

It naively seems like the above offers a solution to our low-energy-problem but the typical problem that arises in scenarios regarding annealings is a crossing of the eigenenergies as a function of time, see figure 11. If such a crossing exists, there is no way of knowing which way the wave function will go without a promise that the spectral projections have the same one-sided right- and left-hand-limits. Therefore, a better choice of annealing Hamiltonian $H_{\text{anneal}}(s)$ would be one with no degeneracies for $s \in (0, 1)$. Could such a Hamiltonian be found, the method would work with certainty. One can use second order perturbation theory to analyze when such a system will have avoided crossings or not [14] but as of now, the construction has no promise of working.

There is also one last thing to consider: Can $H_{\text{anneal}}(s)$ actually be implemented? If $H_{\text{anneal}}(s)$ ends up being more complex than H_{target} then the whole gadget construction loses its usability. All in all, if one were to add an annealing processes to the protocol of applying a Hamiltonian gadget, it seems like the protocol should depend a lot on the system and the concrete gadget one was attempting to construct. Ultimately, the idea of a general annealing implementation seems limited in its universal applicability.

5.2.3 Protocols for testing

The two previous approaches attempted to lead the states that were in the high-energy subspace into a corresponding low-energy part. Another approach one could take is not enforce the promise but to check whether or not it is true and subsequently whether or not the gadget has worked. That is what we will do in the following section.

In all of the gadgets presented, the low-energy subspace is characterized by the state of the ancilla qubit, so it would seem natural to measure this one in a clever way. For the perturbative gadget for instance, a measurement on the ancilla qubit will determine whether the action of

the simulator Hamiltonian is the same as the target Hamiltonian up to error ε or not, totally determined by whether the state of the ancilla is $|0\rangle_m$. But since this is a dynamical operation for which the system has to stay below the energy gap for the duration of application of H_{sim} , the only way to assure that this is always upheld is to continuously measure the ancilla qubit in a Zeno-like-manner. Since the desired dynamics is over the rest of the system, continuous measurement of the ancilla should not change the simulation. Furthermore, by the Quantum Zeno-effect [16], one could even use this to force the ancilla qubit continuously into its ground state.

The same method sadly can't be applied for the Logical gadget, since the low-energy subspace both have support on $|0_m\rangle$ and $|1_m\rangle$, dependent of the state of qubits 1 and 2. A measurement on the ancilla qubit thus won't give us information on whether the process worked or not. Sadly, one also can't just measure both the ancilla and qubits 1 and 2, since this would collapse any superposition that was previously in the system and thus lead to a lack of quantum dynamics in a quantum computer.

One can instead attempt to make a protocol that, with minimum loss of information, leads to enough determination of the system to conclude whether " $N_m = N_1 \wedge N_2$ " is true or not. We will now introduce two such protocols, for which the first has some loss but is surely implementable and the other has no loss but works on a 4-level qudit instead of a qubit.

The first proposal is to use the ancilla qubit m to check whether qubit 1, 2 and m are in the same logical state. Imagine we start in state $|\psi\rangle$ on qubits 1, 2, 3 and m . As an algorithm the protocol would then look like "Protocol 1":

Protocol 1 Test for Low-energy Subspace with Information Loss

Start in state $|\psi\rangle$

Apply $C_1\text{NOT}_m$.

Measure qubit m in computational basis.

If Measurement gives 1:

 Stop algorithm. Algorithm has failed.

Apply $C_2\text{NOT}_m$.

Apply $C_1\text{NOT}_m$.

Measure qubit m in computational basis

If Measurement gives 1:

 Stop algorithm. Algorithm has failed.

Terminate algorithm. Algorithm has succeeded.

The steps until Measurement 1 of the protocol is to check whether qubit 1 has the same value as qubit m . By measuring 0, we will know that they were the same and by measuring 1, we will know that they differed. The steps until Measurement 2 is there to check if qubit 1 and qubit 2 hold the same binary value in the same sense. If both steps succeed, we know that " $N_1 = N_2 = N_m$ ", which implies that the mechanism worked on whatever states we have left after measurement. Sadly, since we learn that the control bits are the same, we have collapsed any branch of the wave function which isn't symmetric under the SWAP-gate on bits 1 and 2. Thus, the protocol introduces a loss of information, but if the wave-function is restricted to the subspace $\text{span}(|0_10_2\rangle, |1_11_2\rangle)$ the protocol works.

Our other proposal for a protocol consists of introducing an extra ancilla qudit m_2 of 4 energy levels. We imagine that we can make a controlled-raising operator with periodic raising property: $C_k a_{m_2}^\dagger$ with $C_k a_{m_2}^\dagger |j\rangle = |\text{mod}(j \oplus k)_4\rangle$. Then we apply the following protocol:

Protocol 2 Test for Low-energy Subspace without Information Loss with 4-level qudit

Start in state $|\psi\rangle|0\rangle_{m_2}$

Apply $C_m a_{m_2}^\dagger$.

Apply $C_m a_{m_2}^\dagger$.

Apply $C_1 a_{m_2}^\dagger$.

Apply $C_2 a_{m_2}^\dagger$.

Measure whether the quantum number is below or above $\frac{3}{2}$.

If we measure the qudit in state $|0_{m_2}\rangle$ or $|1_{m_2}\rangle$, we know that our original state was either $|0_1 0_2 0_m\rangle, |0_1 1_2 0_m\rangle, |1_1 0_2 0_m\rangle$ or $|1_1 1_2 1_m\rangle$ and thus in the low-energy-part of the gadget. If we get $|2_{m_2}\rangle$ or $|3_{m_2}\rangle$ we know that our original state was either $|0_1 0_2 1_m\rangle, |1_1 0_2 1_m\rangle, |0_1 1_2 1_m\rangle$ or $|1_1 1_2 0_m\rangle$, that is, in the high-energy subspace and thus wrong. This protocol should work in the sense that it only "collapses away" the branches of the wave function that either constitute success or failure of applying the gadget. Therefore, it shouldn't introduce loss of information but only a certain answer for whether the gadget worked or not.

In this way, we have introduced two different protocols for how one wouldn't have to force the ancilla qubit into its low-energy subspace in the Logical gadget construction but instead measure cleverly. Sadly, both of these protocols seem unfeasible as the first would collapse away parts of the wave-function and the other would require strong control on a 4-level qudit. Yet these protocols are in no way exhaustive in respect to all strategies one could take, so hopefully there exist possible protocols that succeed at concluding which subspace we're in but are actually feasible to implement.

5.3 Strengths and Weaknesses of Gadgets

We have constructed three types of gadget for analogue Hamiltonian simulation that each have their strengths and weaknesses. We will in this section go over these to give an overview of what each of the gadgets can and can't do.

In terms of weaknesses, the Perturbative and the Logic gadget both only work under the promise of being in the low-energy-subspace of the simulator Hamiltonian. We discussed to great length how one might implement this in a physical system but in the end, these methods lacked operationality; they all failed on some end or another in respect universal applicability. Even after overcoming this hurdle and projecting down to the low-energy-subspace, the Perturbative gadget only works approximately where the Logical gadget works exact, but can only simulate classes of Hamiltonians that are comprised of projectors.

On the contrary, the simulations of the Magnus gadget are exact but only when the heuristics of the method works. Even then, one needs to numerically calculate the parameters of the construction since the expansion is unfeasible to work with analytically. The gadget doesn't produce a recipe for constructing arbitrary interactions and the Magnus expansion becomes drastically more difficult to calculate explicitly as the local complexity and connectivity grows.

Luckily, the gadgets are not without their respective strengths. On the strength side, the perturbative gadget has a power series that very easily inspires how one could simulate arbitrarily locally complex interactions. Thus, if one is willing to accept a sufficient number of counter terms or a considerable margin of error, the gadget provides a straightforward path for how one can simulate interactions of high locality. The backlash of this is of course that the error decays rather slowly and thus, one needs a larger and larger gap for this method to be feasible.

The Logical gadget was shown to be able to represent the logical statement "NAND". By the logical universality of the NAND-logical expression, this shows that one can make just about any logical statement as compositions of the logical gadget. Concretely, by the successive use of AND-gadgets in either series or parallel, we showed that one can get an ancilla qubit to hold the logical AND-statement of many target qubits, and a 2-local interaction with this ancilla will simulate the interaction between every target qubit. This gives a clear recipe for simulating operators of arbitrarily high locality. A drawback of this method is the need for as many ancilla qubits as we have target qubits minus one, see fig 9. Another draw-back of the construction is the need for decoupling each ancilla-qubit after application of the gadget if used to implement a gate.

We showed that the Magnus Gadget could simulate a Toffoli with single 2-local interactions with a time resource improvement on both T_{weak} and T_{strong} in comparison to ordinary decompositions into CNOT's . With the universality of the Hadamard and Toffoli, this should enable us to make any unitary operation from the Magnus Gadget via the universality of the Toffoli Gate Set.

The general strengths and weaknesses of the gadgets are summarized in table 3.

In the next section, we will show applicability of the constructions we have created so far by analyzing them on the real quantum hardware of the QuEra quantum computer.

	Strenghts	Weaknesses
Perturbative gadget	Only uses 1 ancilla. Obvious generalization to higher locality.	Needs Low-Energy-Subspace. Approximative.
Logic gadget	Exact. Logically Universal.	Needs Low-energy Subspace. Needs to decouple. Only projections.
Magnus gadget	Exact. Doesn't need low-energy-subspace. Doesn't need ancillas.	In general hard to analyze. Heuristical.

Table 3: Overview of strengths and weaknesses of each gadget.

6 Application

We have in this thesis introduced three different gadgets that succeed to different extends at simulating Hamiltonians of high locality via operators of low locality. Mainly, it has been at a very theoretical level in the sense that we have attempted to simulate operators via varying connectivities, target Hamiltonians and simulator Hamiltonians. In order to show relevance to a real-life application, we will in the following section attempt to analyse the use of our gadgets onto a real-life analogue quantum computer. Concretely, we will discuss the applicability of the three gadgets on the AWS-QuEra quantum computer, an analogue quantum computer provided by the Amazon Braket quantum computing service. The QuEra-computer utilizes Rydberg atoms for qubits, an atom with large principle quantum number such that it couples strongly to external electric fields. The system furthermore have the intrinsic property of a Rydberg Blockade: An interaction that attempts to not have multiple neighbouring Rydberg atoms in the excited state [19]. Besides this inherent interaction in the system, the framework of the computer allows one to apply time-dependent electric pulses to make global on-site potentials. The over-all time-dependent Hamiltonian of QuEra can thus be parameterized as [19]:

$$H_{\text{QuEra}}(t) = \sum_i \frac{\Omega(t)}{2} (e^{i\phi(t)} |0\rangle \langle 1|_i + \text{h.c.}) - \sum_i \Delta(t) N_i^z + \sum_{j>i} V_{ij} N_i^z N_j^z$$

Where the interaction strengths are given as:

$$V_{ij} = \frac{C_6}{|r_i - r_j|^6}$$

With $C_6 = 2\pi \times 862690 \text{ MHz } \mu\text{m}^6$ and where r_i is the position of the i 'th Rydberg atom interpreted as a classical object with fixed position. Notice that the Rydberg blockade is always non-zero and therefore will couple all atoms pairwise. Notice furthermore that the on-site pulses $\Omega(t)$ and $\phi(t)$ are global in the sense that they act the same on all atoms.

We will redefine the activation pulses of QuEra as:

$$u^x(t) \equiv \frac{\Omega(t)}{2} \cos(\phi(t)), \quad u^y(t) \equiv \frac{\Omega(t)}{2} \sin(\phi(t)), \quad u^z(t) \equiv -\frac{\Delta(t)}{2}$$

So the Hamiltonian instead becomes of the form:

$$H_{\text{QuEra}}(t) \simeq \sum_i u^x(t) X_i + u^y(t) Y_i + u^z(t) Z_i + \sum_{j>i} V_{ij} N_i^z N_j^z$$

Here we have removed terms proportional to the identity since they don't change dynamics. This form of the Hamiltonian helps to make application of each of the three gadget more transparent and evident in their results. We will in the following sections apply the three gadgets and see what we can get out of them.

6.1 Perturbative Gadget

We will in this section use the Perturbative gadget to approximately simulate a 3-local interaction with all-to-all $Z_i Z_j Z_k$ connectivity on the QuEra hardware. We will begin by discussing which strategies for the Perturbative gadget are feasible and then find out which simulation we get out of this construction.

The formulation of the Perturbative gadget we have so far done in this thesis consists of applying a large on-site potential on a single ancilla qubit to define the high- and low-energy subspaces. The framework of QuEra isn't well suited for this version of the Perturbative gadget since the on-site Hamiltonians are global. This means that it isn't possible to define the low-energy subspace via a single ancilla qubit. In contrary, a global large onsite potential would force the low-energy subspace to be the space for which every bit aligns with the on-site potential. By doing so, we ensure that no further dynamics can occur, since no qubit can change state without moving out of the low-energy subspace.

One could instead put two qubits really close to each other and let their Rydberg Blockade-energy wall constitute the ancilla with an energy gap. Sadly, the part of the Hamiltonian which excites or relaxes in and out of this subspace are the global on-site potentials. These terms don't couple atoms to each other and thus won't produce exciting dynamics to lowest order in the perturbative expansion.

A viable application of the gadget exists as a combination of both of these ideas for low-energy-subspaces. Thus, we will use two ancilla qubits with a large Rydberg Blockade together with an on-site potential to define the unperturbed Hamiltonian. The decomposition into high- and low-energy-subspaces will thus be defined via a Hamiltonian of the form:

$$H_0 = \Omega (X_{m_1} + X_{m_2}) + \Delta N_{m_1}^z N_{m_2}^z$$

Where we define the strength of the on-site potential Ω and a gap parameter $\Delta \equiv V_{m_1 m_2}$ which we expect to be very large. Before the application of the on-site Rabi-term, the low-energy-subspace was the span of the three states $|0_{m_1} 0_{m_2}\rangle, |0_{m_1} 1_{m_2}\rangle, |1_{m_1} 0_{m_2}\rangle$, each with eigenvalue 0 and the high-energy-subspace consisted of the span of the single vector $|1_{m_1} 1_{m_2}\rangle$. The Rabi-term lifts the degeneracy but also rotates the eigenstates, such that the eigenvectors aren't eigenstates of $N_{m_1}^z N_{m_2}^z$ anymore. To simplify the calculation of the self-energy, we call the high-energy-eigenvector $|v\rangle$ and denote the following objects:

$$\begin{aligned} P_+ &= |v\rangle \langle v| \\ P_- &= \mathbb{1} - |v\rangle \langle v| \\ |w\rangle &\equiv (N_{m_1}^z + N_{m_2}^z) |v\rangle \end{aligned}$$

We have that $P_- |w\rangle \neq 0$ unlike before we added the on-site X -term. Now we are in a position in which the Perturbative gadget can actually be utilized.

We apply a perturbation which corresponds to adding more Rydberg Atoms to the system that couples to our ancilla:

$$V = (N_{m_1}^z + N_{m_2}^z) \sum_i V_{im} N_i^z \equiv N \sum_i V_{im} N_i^z$$

Where $N \equiv N_{m_1}^z + N_{m_2}^z$. Notice that we made the geometric approximation that $V_{mi} \equiv V_{m_1i} \approx V_{m_2i}$, which only holds since the two ancilla qubits are close together to make the large energy gap. We redefine our starting Hamiltonian to also hold the interaction terms that are present on QuEra when adding more atoms:

$$H_0 = \Omega (X_{m_1} + X_{m_2}) + \Omega \sum_i X_i + \Delta N_{m_1}^z N_{m_2}^z + \sum_{j>i} V_{ij} N_i^z N_j^z$$

As long as $\Delta > n\Omega + \sum_{j>i} V_{ij}$ where n is the total amount of particles, the high and low-energy-subspaces remain unchanged. From this we get the building blocks:

$$\begin{aligned} V_{--} &= P_- N P_- \sum_i V_{im} N_i^z = N_{--} \sum_i V_{im} N_i^z \\ V_{+-} &= (V_{-+})^\dagger = P_+ N P_- \sum_i V_{im} N_i^z = N_{+-} \sum_i V_{im} N_i^z \\ V_{++} &= P_+ N P_+ \sum_i V_{im} N_i^z = N_{++} \sum_i V_{im} N_i^z \end{aligned}$$

Like we have previously done, we must write up the self-energy of this system, which to third order becomes:

$$\begin{aligned} \Sigma(z) &= (H_0 + V)_{--} + \frac{V_{-+} V_{+-}}{z - \Delta} + \frac{V_{-+} V_{++} V_{+-}}{(z - \Delta)^2} + \dots \\ &= (H_0 + V)_{--} + N_{-+} N_{+-} \frac{(\sum_i V_{im} N_i^z)^2}{z - \Delta} + N_{-+} N_{++} N_{+-} \frac{(\sum_i V_{im} N_i^z)^3}{(z - \Delta)^2} + \dots \end{aligned}$$

We can make the small calculation:

$$\begin{aligned} N_{-+} &= (N_{+-})^\dagger = P_- N P_+ = P_- (N_{m_1}^z + N_{m_2}^z) |v\rangle \langle v| = P_- |w\rangle \langle v| \\ N_{++} &= P_+ N P_+ = |v\rangle \langle v| (N_{m_1}^z + N_{m_2}^z) |v\rangle \langle v| = |v\rangle \langle v| \cdot \langle v|w\rangle \end{aligned}$$

We see that the order of every term in the geometric series of the self-energy depends on the objects $N_{-+} \sim P_- |w\rangle$ and $N_{++} \sim \langle v|w\rangle$ and that the first order term depends on $N_{--} = P_- N P_-$. An essential question to the convergence of the series is then how these scale as Δ increases. This is easier simulated than calculated, given that the characteristic polynomial of this problem is lengthy and an analytical nightmare. The results of these numerics are shown in figure 12.

In figure 12 one can see $\|P_- |w\rangle\|$, $\langle v|w\rangle$ and $\|P_- N P_-\|$ as a function of $\frac{\Delta}{\Omega}$. We see that $\langle v|w\rangle$ converges to 2 rapidly which corresponds to the high-coupling regime for which the high-energy

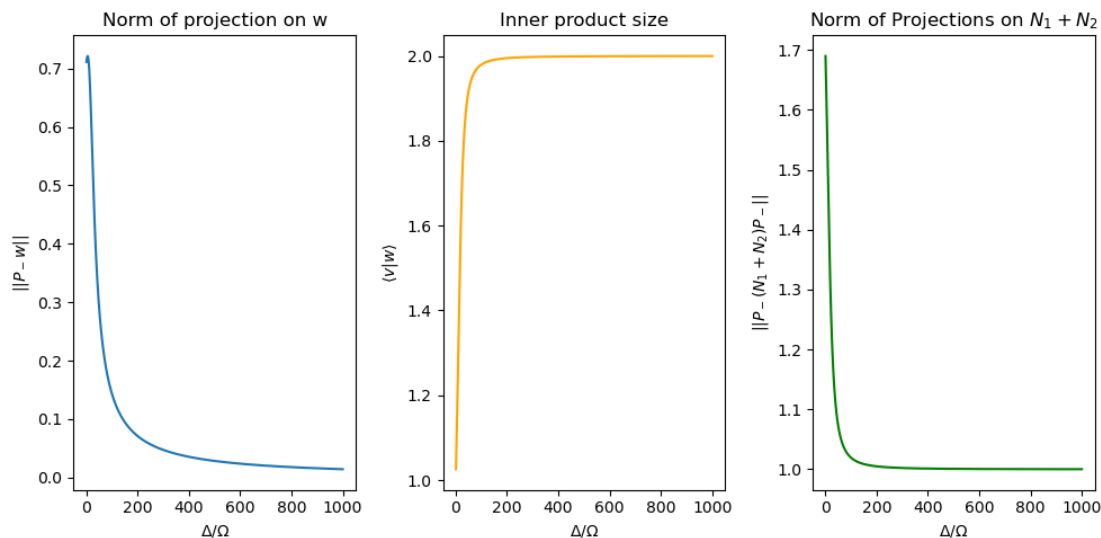


Figure 12: The norm of $P_-|w\rangle$, the overlap $\langle v|w\rangle$ and the norm of $P_-(N_{m_1}^z + N_{m_2}^z)P_-$ as a function of Δ/Ω . We see that the first decays, whilst the second and third rapidly becomes 2 and 1, corresponding to $|w\rangle = 2|v\rangle$ and $|v\rangle \approx |11\rangle$ in the high- ZZ -coupling-regime. The first graph has been fitted to a first order regression on a log-log-scale and produce a slope of $a = -1.004$.

subspace has the property: $|w\rangle = (N_{m_1}^z + N_{m_2}^z)|v\rangle \approx 2|v\rangle$, since $|v\rangle \approx |11\rangle$. In this regime we also get that $P_-(N_{m_1}^z + N_{m_2}^z)P_- \approx |0_{m_1}1_{m_2}\rangle\langle 0_{m_1}1_{m_2}| + |1_{m_1}0_{m_2}\rangle\langle 1_{m_1}0_{m_2}|$, becomes of norm 1, which explains the third plot.

We fit the decay of $\|P_-|w\rangle\|$ to fall off like $\|P_-|w\rangle\| \sim \Delta^a$ with $a = -1.004$, and we'll assume asymptotically that $a = -1$ in the following section. This is really bad news for the hope of a stable perturbative gadget, since every term in the self-energy has a factor of V_{-+} and V_{+-} . To clarify, the n 'th order term will be divided by $(z - \Delta)^{n-1}$ from the resolvent in the geometric series but also have a factor of Δ^{-2} from $V_{-+}V_{+-}$. Thus every term will at best decay two orders of Δ faster than if V_{-+} was increasing in Δ like it has been for previous Perturbative gadget constructions.

This means that asymptotically we get:

$$\Sigma(z) = (H_0 + V)_{--} + |q\rangle\langle q| \frac{(\sum_i V_{im} N_i^z)^2}{\Delta^2(z - \Delta)} + |q\rangle\langle q| \frac{2(\sum_i V_{im} N_i^z)^3}{\Delta^2(z - \Delta)^2} + \dots$$

Where $|q\rangle \equiv \frac{P_-|w\rangle}{\|P_-|w\rangle\|}$ and the factor of 2 on the third order term comes from $\langle v|w\rangle$. It isn't possible to choose V_{im} large enough to cancel the energy gap in the denominator on either of the terms without the perturbation breaking down. Thus for any finite Δ , the Perturbative gadget works to some error ε , but to make this error arbitrarily small would also be to make the

interesting dynamics we attempt to simulate equally small.

We can analyse the error better by calculating the rest of the terms in the self-energy exactly:

$$\begin{aligned}
 \Sigma(z)_{n \geq 4} &\equiv \sum_{k=2}^{\infty} \frac{V_{-+} V_{++}^k V_{+-}}{(z - \Delta)^3} \\
 &= \sum_{k=0}^{\infty} P_- |w\rangle \langle w| P_- \frac{(\langle v|w\rangle)^{k+2} (\sum_i V_{im} N_i^z)^{k+4}}{(z - \Delta)^{k+3}} \\
 &= P_- |w\rangle \langle w| P_- (\langle v|w\rangle)^2 \frac{(\sum_i V_{im} N_i^z)^4}{(z - \Delta)^3} \sum_{k=0}^{\infty} \left(\frac{\langle v|w\rangle \sum_i V_{im} N_i^z}{z - \Delta} \right)^k \\
 &= P_- |w\rangle \langle w| P_- (\langle v|w\rangle)^2 \frac{(\sum_i V_{im} N_i^z)^4}{(z - \Delta)^3} \frac{z - \Delta}{z - \Delta - \langle v|w\rangle \sum_i V_{im} N_i^z}
 \end{aligned}$$

The last equality sign is conditioned on the assumption that the sum converges, which is true by the perturbation not breaking down ($\Delta \geq \frac{\|V\|}{2}$). If the interaction strengths V_{im} are kept constant, this grows asymptotically like $O(\Delta^{-5})$ to constant order in z .

In conclusion, we can look at the self-energy from above and expand to first order in z to simulate the target Hamiltonian:

$$\begin{aligned}
 H_{\text{target}} &= P_- (\Omega X_{m_1} + \Omega X_{m_2}) P_- + \Omega \sum_i X_i + \sum_{j>i} V_{ij} N_i^z N_j^z + P_- (N_{m_1}^z + N_{m_2}^z) P_- \left(\sum_i V_{mi} N_i^z \right) \\
 &\quad - |q\rangle \langle q| \frac{\|P_- |w\rangle\|^2}{\Delta} \left(\sum_i V_{im} N_i^z \right)^2 + |q\rangle \langle q| \langle v|w\rangle \frac{\|P_- |w\rangle\|^2}{\Delta^2} \left(\sum_i V_{im} N_i^z \right)^3
 \end{aligned}$$

The error on the rest of the self-energy is $\varepsilon = O(\Delta^{-5})$ to zeroth order in z , whilst the error from terms we have already expanded in z to first order becomes $\varepsilon = O(\Delta^{-4})$ which therefore dictates the order of the total error.

We've solved the problem we sought out to do: To apply the perturbative gadget to the QuEra framework and find a Hamiltonian of interest that can be simulated approximately. The Hamiltonian we found was one that, amongst many other terms, simulated all-to-all-three body $Z_i Z_j Z_k$ -couplings, which is much like the interaction QuEra already have built in but as a 3-local operator instead of a 2-local one.

Since the interesting part of the interaction scales with the energy gap, one needs to spend longer time in order to get interesting dynamics in the time-evolution operator. As an initial estimate, we should require something like $t \sim \Delta^4$ since the third order term has a norm that scales like Δ^{-4} . But a short calculation via the fundamental theorem of calculus shows that we could run into an issue:

$$\|U_{\text{sim}} - U_{\text{target}}\| = \left\| \int_0^t \frac{d}{ds} \exp(-is(H_{\text{sim}} - H_{\text{target}})) ds \right\| \leq \|H_{\text{sim}} - H_{\text{target}}\| t \sim \frac{1}{\Delta^4} \Delta^4 = 1$$

So the accuracy of the simulation of the Hamiltonian doesn't produce a naive promise that the accuracy of the time evolution actually does go down.

Thus, we succeeded at approximately simulating a 3-local Hamiltonian on the QuEra Hardware under the promise of being in the low-energy-subspace but without necessarily simulating its time-evolution in a valuable way.

There are multiple things one can criticize this simulation for. One of them is the same as in the section 5.2: How can one make sure that we are confined to the low-energy-subspace? Here the promise is equivalent to forcing qubits m_1 and m_2 into the orthogonal complement of $|v\rangle$ but the interesting dynamics only occur as long as they exist within $\text{span}(|w\rangle)$ which comes really close to $|v\rangle$ as Δ increases. Thus, it is an even harder requirement than previously to actually simulate exciting dynamics. Even after this obstacle has been overcome, the simulated interaction does include third-order interactions, but it is amidst many more terms of little interest that aren't decaying in size for increasing Δ . Thus, the predominant part of the target Hamiltonian just looks like the simulator Hamiltonian itself, added a term of small norm but higher locality.

This construction should not be understood as a major success but we will in the following section discuss the Logical gadget, which is much better suited for the QuEra computer and thus has a better chance at succeeding.

6.2 Logical Gadget

We will in the following section simulate a 3-local interaction on QuEra via the Logical gadget. The framework of QuEra intuitively seems like it is well-suited for the Logical gadget construction: Its main constituent is a bunch of interaction terms that are 2-local products of projections which is exactly the starting point of the Logical gadget. The key shortfall in the framework is the lacking possibility to add a product of projections with a negative or zero weight. On the QuEra hardware, only the on-site potentials can have negative weights and thus, one needs to be creative in order to get the proper frustration between relevant qubits such that the low-energy-subspaces are equivalent to the fulfillment of logical statements.

There exists an easy construction from the framework which utilizes the building blocks that is inherent in QuEra: The Rydberg Blockade. The qualitative description of this physical phenomenon is exactly a tendency not to have two qubits close to one another excited at the same time. Naturally, this can be reformulated as a logical condition in the form of the “not-link”

$$H_{\text{not-link},1\leftrightarrow 2} = -\Delta(N_1^z - N_2^z)^2 = \Delta(N_1^z N_2^z - N_1^z - N_2^z)$$

This penalty Hamiltonian exactly has the property that its low-energy-subspace is governed by states for which “ $N_1 \neq N_2$ ”. The sum of many “not-links” become a “not-chain”, which can be used to convey logical bits over long distances in the same sense that the chain-gadget could in section 4.2.

This is a very natural use of the Rydberg Blockade. QuEra has also pointed this out themselves and have worked further on such constructions [22]. They have for instance made the “NOR”-statement “ $N_1 = \neg(N_2 \vee N_3) = (\neg N_1) \wedge \neg(N_2)$ ” as the low-energy-spectrum of the Hamiltonian

acting on three target qubits and two ancilla qubits:

$$H_{\text{NOR}} = U(N_1^z N_2^z + N_2^z N_{m_1}^z + N_{m_1}^z N_{m_2}^z + N_{m_2}^z N_3 + N_3^z N_1^z) - \delta(N_1^z + N_2^z + N_3^z + N_{m_1}^z + N_{m_2}^z)$$

Where m_1 and m_2 are ancilla qubits and U and δ are parameters that correspond to some positions of the atoms and biases on them. This construction works as long as $U > \delta$, which is equivalent to saying as long as the Rydberg Blockade is energetically favored over the onsite potential. The degenerate ground-state exactly produces the frustration that has excited qubit 1 if and only if both qubit 2 and 3 aren't excited. By the logical universality of the NAND-operation, compositions of this Hamiltonian can make any logical statement, given enough ancilla qubits [22].

Thus if one imagines we apply the above Hamiltonian as a penalty where we interpret N_2 and N_3 as free parameters whilst the eigenvalues of N_1, N_{m_1} and N_{m_2} are fixed to lower the energy then the interaction:

$$H_{\text{sim}} = H_{\text{int}} + H_{\text{NOR}} \equiv V_{41} N_4^z N_1^z + H_{\text{NOR}}$$

is a Logical gadget much like the AND-Logical gadget. As long as V_{41} is negligible in respect to both U and δ , the low-energy-subspace is still characterized by the statement “ $N_1 = (\neg N_2) \wedge (\neg N_3)$ ”. Thus the interaction term perfectly simulates the interaction $H_{\text{target}} = N_4^z \overline{N_3^z} \overline{N_2^z}$ under the promise of staying in the low-energy subspace.

Now, even though the above construction does simulate an interaction of interest, we must notice that the hardware from QuEra actually can't implement the NOR-Hamiltonian, since it doesn't have all-to-all connectivity. But by loosening the demand from “the logical statement is embedded in the ground-state” as QuEra have done in their work to “the logical statement is embedded in the low-energy-subspace”, we can make a simplified toy-version of the NOR-penalization term:

$$H_{\text{toy}} = U(N_1^z N_m^z + N_2^z N_m^z + c N_1^z N_2^z) - \delta(N_1^z + N_2^z + N_m^z)$$

Here, c is some number $0 < c < 1$ that represent having placed qubits 1 and 2 further from each other than from the ancilla qubit. This toy-Hamiltonian is obviously diagonalized in the standard basis and its spectrum with corresponding eigenvectors is written in table 4.

We can see from table 4 that as long as $2 \leq \frac{U}{\delta} \leq \frac{2}{c}$, all states that fulfill “ $N_m = (\neg N_1) \wedge (\neg N_2)$ ” have negative energy, whilst all other states have positive (or zero) energy. The energy gap between the two subspaces $\Delta = 2\delta - cU$ becomes larger for increasing δ with fixed c and U or decreasing U for fixed δ and c .

This prepares us to make the following kind of interaction:

$$H_{\text{sim}} = H_{\text{int}} + H_{\text{toy}} \equiv V_{31} N_3^z N_1^z + V_{32} N_3^z N_2^z + V_{3m} N_3^z N_m^z + H_{\text{toy}}$$

Eigenstates	Energies of H_{toy}
$ 0_1 0_2 0_m\rangle$	0
$ 0_1 0_2 1_m\rangle$	$-\delta$
$ 0_1 1_2 0_m\rangle$	$-\delta$
$ 0_1 1_2 1_m\rangle$	$U - 2\delta$
$ 1_1 0_2 0_m\rangle$	$-\delta$
$ 1_1 0_2 1_m\rangle$	$U - 2\delta$
$ 1_1 1_2 0_m\rangle$	$cU - 2\delta$
$ 1_1 1_2 1_m\rangle$	$(2 + c)U - 3\delta$

Table 4: Energies of the different eigenstates of H_{toy} . Here a logical 0_k means that $N_k |0_k\rangle = 0$ and a logical 1_k means that $N_k |1_k\rangle = |1_k\rangle$.

This is a Logical gadget that, in its low-energy subspace, simulates the target Hamiltonian:

$$H_{\text{target}} = V_{31} N_3^z N_1^z + V_{32} N_3^z N_2^z + V_{m3} N_3^z \overline{N_2^z N_1^z} + P_- H_{\text{Toy}} P_-$$

Which is an effective 3-body-interaction added to two 2-body interactions. We can make the toy-part trivial by choosing parameters U, δ and c such that $cU = \delta$. Then we have:

$$P_- H_{\text{toy}} P_- = -\delta \cdot P_-$$

Under the promise of staying in the low-energy subspace, a term that is proportional to the projection onto the low-energy subspace acts as a multiple of the identity. This means that the target Hamiltonian, up to irrelevant multiples of the identity, becomes:

$$H_{\text{Target}} \simeq V_{31} N_3^z N_1^z + V_{32} N_3^z N_2^z + V_{3m} N_3^z \overline{N_2^z N_1^z}$$

This is as close as we can get to a bare 3-qubit interaction in the QuEra-framework via the Logical gadget. One could attempt to put such gadgets in series or parallel like with the general Logical gadget, but such constructions will fail given their lack of all-to-all-connectivity; a property that is unavoidable in the QuEra framework. It seems like the adventure ends here for the Logical gadget as long as there is no way to cleverly manipulate the Rydberg Blockade.

Thus, by the success of this toy-Hamiltonian, we can succeed in simulating Hamiltonians of larger locality. Sadly, any Hamiltonian we can simulate in this manner will be diagonal in the Z -basis, and thus can't create non-classical dynamics alone. The only resource we have access to which isn't diagonal in the standard basis is the on-site biases and they are restricted both by only being on-site and by being global for the whole system. Thus, the Logical gadget worked well at simulating non-local target Hamiltonians but the simulations were sadly dynamically uninteresting alone.

We have so far not utilized the possibility of time-dependence in the QuEra framework. This is due to the Perturbative and Logical gadgets being time-independent in their construction but in the following section, we will attempt to utilize this degree of freedom in the simulation via the Magnus gadget.

6.3 Magnus Gadget

We will in the following section attempt to utilize the Magnus gadget heuristic onto the QuEra Hamiltonian to produce 3-local interactions. Sadly, the framework of QuEra is badly suited for the Magnus gadget, mainly because time dependencies only can be implemented in global on-site interactions. Thus, it becomes impossible to distinguish strongly between ancilla and target qubits in the interactions one wants to simulate. On the other hand, all interaction terms are products of projections which is partially the same form as the constructions made in section 4.3.

We will use the example of only two atoms to gain insight on the situation. If we prepare two atoms in the QuEra machine then we'll be preparing a Hamiltonian of the form:

$$H(t) = u^x(t)(X_1 + X_2) + u^y(t)(Y_1 + Y_2) + u^z(t)(Z_1 + Z_2) + V_{12}N_1^z N_2^z$$

To make the situation as simple as possible, we will make the pulse in the form:

$$H(t) = u(t)(Y_1 + Y_2) + V_{12}Z_1 + V_{12}Z_2 + 4V_{12}N_1^z N_2^z \simeq u(t)(Y_1 + Y_2) + V_{12}Z_1 Z_2$$

This is one of the simplest implementable forms of a time-dependent Hamiltonian which produces non-trivial dynamics in its Magnus expansion. By application of successive commutators, we see that:

$$\Omega_1 \in \text{span}(Y_1, Y_2, Z_1 Z_2)$$

$$\Omega_2 \in \text{span}(X_1 Z_2, Z_1 X_2)$$

$$\Omega_3 \in \text{span}(Z_1 Z_2, X_1 X_2, Y_1 Z_2, Z_1 Y_2)$$

We can already see that we produce practically all kinds of possible interaction terms, since the group of operators that are closed under taking commutators with the Hamiltonian is a huge set. The heuristics of the method tells us that making the pulse $u(t)$ be symmetric around the mid-point will kill off the terms of the form XZ . Though it's not clear which of the remaining terms will have non-zero weight.

Concretely, if we make the following pulse for a period of $T = \pi$:

$$H(t) = a \cos(4t)(Y_1 + Y_2) + bZ_1 Z_2$$

with amplitudes a and b , we get that the Magnus expansion to third order becomes:

$$\begin{aligned}\Omega_1 &= -i \int_0^\pi a \cos(4t)(Y_1 + Y_2) + bZ_1Z_2 dt = -ib\pi Z_1Z_2 \\ \Omega_2 &= -iab \int_0^\pi \int_0^{t_1} \cos(t_1) - \cos(t_2) dt_2 dt_1 (X_1Z_2 + Z_1X_2) \stackrel{*}{=} 0 \\ \Omega_3 &= -\frac{2ia^2b}{3} \int_0^\pi \int_0^{t_1} \int_0^{t_2} \cos(t_1) \cos(t_2) - 2 \cos(t_1) \cos(t_3) + \cos(t_3) \cos(t_2) dt_3 dt_2 dt_1 (X_1X_2 - Z_1Z_2) \\ &\quad - \frac{2iab^2}{3} \int_0^\pi \int_0^{t_1} \int_0^{t_2} 2 \cos(t_2) - \cos(t_3) - \cos(t_1) dt_3 dt_2 dt_1 (Y_1Z_2 + Z_1Y_2) \\ &= -i\pi a^2b(X_1X_2 - Z_1Z_2)\end{aligned}$$

Where the $*$ indicates that this equality is true because we required $u(t)$ to be symmetrical. So to third order, we get that the gadget produces an interaction that is the sum of an XX - and a ZZ -term.

This is very fine to give intuition, but we will have to simulate this to arbitrary order to get the full target Hamiltonian, which is what we will do now. We simulate the time-evolution numerically via the QuTip library and take its matrix logarithm to get a target Hamiltonian. Astoundingly, we find that we get the following decomposition of the target Hamiltonian for every choice of a and b :

$$H_{\text{target}} = c_y(Y_1 + Y_2) + c_x X_1 X_2 + c_z Z_1 Z_2$$

We sweep the parameter space (a, b) and find the coefficients c_x, c_y, c_z from the Pauli-decompositions we get. See figure 13 for this numerical simulation.

For $a = 1.23$ and $b = 6.85$, we see from figure 13 that $c_x = 2.6845$ and $c_z = 0$. In conclusion, it seems like it is possible to create the "bare"- XX -interaction together with two on-site Y -pulses. This is of course only a toy-example of 2 atoms, but it still warrants hope for being able to make any 2-local interaction on the QuEra-hardware.

If we do add an extra atom, such that we implement a Hamiltonian of the form:

$$H(t) = u^y(t)(Y_1 + Y_2 + Y_3) + V_{12}Z_1^z Z_2^z + V_{13}Z_1^z Z_3^z + V_{23}Z_2^z Z_3^z$$

The heuristic of the Magnus gadget becomes unfeasible to calculate, since the successive commutators will produce a span of Pauli operators that is huge. Unless we can apply local on-site potentials or turn off the Rydberg Blockade, this seems like an issue that is practically impossible to overcome. Thus it appears as though the Magnus gadget heuristic doesn't go a long way in the QuEra framework when not working with only two atoms, even if the two atom example did show promise of being calculable.

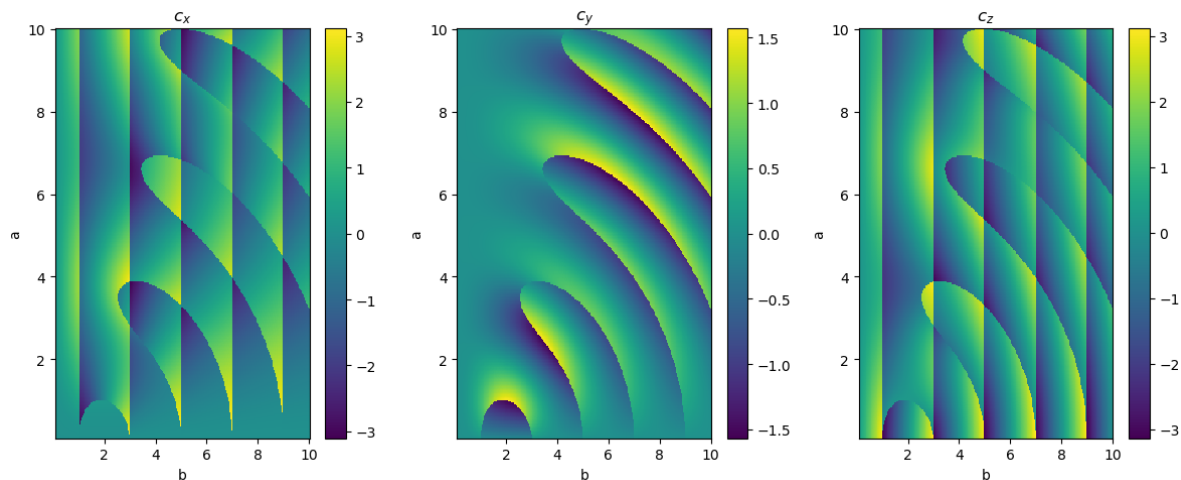


Figure 13: c_x , c_y and c_z as a function of a and b for the construction above.

6.4 Improved QuEra: Local on-site interactions.

We managed to apply our three gadgets to the QuEra framework with varying degrees of success. The Perturbative gadget simulated a three-local interaction amidst a zoo of other terms with a 3-local part of the interaction that decreased in size for increasing accuracy. The Logical gadget succeeded in simulating an almost bare 3-local interactions but with uninteresting, diagonal dynamics. Lastly, the Magnus gadget heuristic was unfeasible to analyze for more atoms than two.

One could now ask oneself: How much better would these constructions yield if one changed the QuEra framework slightly? Concretely, we will in the following sections analyze how much stronger the simulations work if the on-site potentials of the framework acted locally on qubits instead of globally. That is we imagine we can implement Hamiltonians of the form:

$$H(t) = \sum_i u_i^x(t) X_i + u_i^y(t) Y_i + u_i^z(t) Z_i + \sum_{j>i} V_{ij} N_i^z N_j^z$$

With atom-indexed pulses $u_i^x(t)$, $u_i^y(t)$, $u_i^z(t)$. We will in the following section construct gadgets of all three kinds with this imagined improvement on QuEra and end off with a side note of how close the QuEra framework is to have universal simulability in the Cubitt et al. framework.

6.4.1 Perturbative gadget: What if?

On-site control makes the Perturbative gadget a lot easier to construct naturally. Let the ancilla qubit have low- and high-energy subspaces defined by:

$$H_0 = \Delta X_m$$

Add a perturbation that corresponds to coupling the other atoms to your ancilla:

$$V = \sum_i V_{mi} N_i^z N_m^z + \sum_{j>i} V_{ij} N_i^z N_j^z$$

With condition $2\Delta > \sum_{j>i} V_{ij} + \sum_i V_{mi}$ such that the perturbation doesn't break down. Only N_m^z excites and relaxes the ancilla. The relevant operators are thus:

$$\begin{aligned} V_{++} &= (N_m^z)_{++} \sum_i V_{mi} N_i^z + \sum_{j>i} V_{ij} N_i^z N_j^z \mathbb{1}_{++} = \left(\frac{1}{2} \sum_i V_{mi} N_i^z + \sum_{j>i} V_{ij} N_i^z N_j^z \right) |-\rangle \langle -|_m \\ V_{--} &= (N_m^z)_{--} \sum_i V_{mi} N_i^z + \sum_{j>i} V_{ij} N_i^z N_j^z \mathbb{1}_{--} = \left(\frac{1}{2} \sum_i V_{mi} N_i^z + \sum_{j>i} V_{ij} N_i^z N_j^z \right) |+\rangle \langle +|_m \\ V_{+-} &= (N_m^z)_{+-} \sum_i V_{mi} N_i^z = \left(-\frac{1}{2} \sum_i V_{mi} N_i^z \right) |-\rangle \langle +|_m \end{aligned}$$

So to third order in the perturbation, the self-energy becomes:

$$\Sigma(z) = \left(\frac{1}{2} \sum_i V_{mi} N_i^z + \sum_{j>i} V_{ij} N_i^z N_j^z + \frac{(\sum_i V_{mi} N_i^z)^2}{4(z - \Delta)} + \frac{(\sum_i V_{mi} N_i^z)^2 \left(\frac{1}{2} \sum_i V_{mi} N_i^z + \sum_{j>i} V_{ij} N_i^z N_j^z \right)}{4(z - \Delta)^2} \right) |+\rangle \langle +|_m + \dots$$

Which seems a lot closer to the constructions we have made ourselves in this thesis. A natural strategy from here is to use a 3-to-2-gadget inspired construction.

We can simulate a 4-local interaction by choosing each interaction strength $V_{im} = \Delta^\alpha$ and $V_{ij} = c_{ij} \Delta^\alpha$ for some $c_{ij} > 0$ and exponent $0 < \alpha < 1$. Observe that the exponent must be consistent across each term, as they correspond to a scaling of distances. Moving each target qubit halfway towards the ancilla implies moving halfway towards every other target qubit. The c_{ij} 's represent that the target qubits have some distance from each other that is different from their distance to the ancilla qubit. We will as a first approximation put $c_{ij} = c$ for some constant c for all i and j , which of course isn't geometrically possible, but make the following calculation easier.

The first order terms of the self-energy become an on-site bias and a Rydberg Blockade with large weights:

$$\frac{1}{2} \sum_i V_{mi} N_i^z + \sum_{j>i} V_{ij} N_i^z N_j^z = \frac{\Delta^\alpha}{2} \sum_i N_i^z + c \Delta^\alpha \sum_{j>i} N_i^z N_j^z$$

The second order term in the self-energy looks like a Rydberg blockade but with a negative sign:

$$\frac{(\sum_i V_{mi} N_i^z)^2}{4(z - \Delta)} = -\frac{\Delta^{2\alpha-1}}{4} \left(\sum_i N_i^z \right)^2 + O(z \Delta^{2\alpha-2})$$

And the third order term in the self-energy would simulate the 4-local interaction:

$$\frac{(\sum_i V_{mi} N_i^z)^2 \left(\frac{1}{2} \sum_i V_{mi} N_i^z + \sum_{j>i} V_{ij} N_i^z N_j^z \right)}{(z - \Delta)^2} = \Delta^{3\alpha-2} \left(\sum_i N_i^z \right)^2 \left(\frac{1}{2} \sum_i N_i^z + c \sum_{j>i} N_i^z N_j^z \right) + O(z \Delta^{3\alpha-3})$$

The rest of the series should be interpreted as error terms. In this manner, by Theorem 1 we will simulate the 4-local interaction:

$$H_{\text{target}} = \frac{\Delta^\alpha}{2} \sum_i N_i^z + c\Delta^\alpha \sum_{j>i} N_i^z N_j^z - \Delta^{2\alpha-1} \left(\sum_i N_i^z \right)^2 + \Delta^{3\alpha-2} \left(\sum_i N_i^z \right)^2 \left(\frac{1}{2} \sum_i N_i^z + c \sum_{j>i} N_i^z N_j^z \right)$$

All in all, the framework of the Perturbative gadget is a lot easier to construct, given that one has strong single qubit control. But this simulation is far from a success. An issue that we can't overcome is the fact that our target Hamiltonian scales with Δ . This induces the problem we also discussed in section 4.1.4 concerning the direct-k-local-gadget: To achieve a Δ -independent target Hamiltonian, one must incorporate counter terms. Without them, the error scales significantly worse. In the above construction, we have that z can run up to $\|H_{\text{target}}\| = O(\Delta^\alpha)$ from the first order term, the second order term produces an error of $\varepsilon = O(z\Delta^{2\alpha-2}) = O(\Delta^{3\alpha-2})$ to first order in z , which has the same magnitude as the dynamically interesting third-order term. Thus, we either have an error that doesn't decrease for increasing Δ or a third-order term and an error that decrease equally rapidly for increasing Δ . Sadly, the QuEra framework doesn't have the luxury of counter terms and the construction ends its applicability here.

6.4.2 Logical gadget: What if?

Our application of the Logical gadget would not gain anything from having local on-site interactions in itself. The main contributor to stronger constructions would be the possibility to have negative or zero weight on the Rydberg Blockade. Though with an on-site interaction, the dynamics of the simulation of the Logical gadget construction could become a lot more interesting. We were previously able to simulate the interaction:

$$H_{\text{target}} = V_{31} N_3^z N_1^z + V_{32} N_3^z N_2^z + V_{3m} N_3^z \overline{N_2^z N_1^z}$$

To make this simulation more interesting, we will imagine we could apply a pulse onto qubit 3 of the form of a Hadamard H_1 , that is $H_{\text{pulse}} = aH_3 = \frac{a}{\sqrt{2}}(X_3 + Z_3)$ where a is so large that the Rydberg Blockade will be negligible during the time the pulse active. It should last for a period of $t = \frac{\pi}{2a}$ such that we get a time evolution of a Hadamard up to a global phase $U(t) = \exp(-itH_{\text{pulse}}) = -iH_{\text{pulse}} = -iH_3$. Then, our new simulated Hamiltonian $\tilde{H}_{\text{target}}$ would become:

$$\tilde{H}_{\text{target}} = (U(t))^\dagger H_{\text{target}} U(t) = V_{31} N_3^x N_1^z + V_{32} N_3^x N_2^z + V_{3m} N_3^x \overline{N_2^z N_1^z}$$

Which, if we neglect the first two terms, is the "not-control-not-control-flip"-interaction; a modified Toffoli that flips the third qubit if and only if the two first are in the 0-state. So if one gets strong enough 1-local control to be able to apply pulses in a manner such that the Rydberg Blockade can become negligible, one can almost create a not-control-not-control-flip gate. Sadly

from the condition that $0 < c < 1$ of the toy-Hamiltonian in the simulator, we get from the geometry that this implies that $V_{31} \geq \frac{1}{8}V_{3m}$ and $V_{32} \geq \frac{1}{8}V_{3m}$ and thus, these terms can't be made negligible in a strong sense. But the Logical gadget did manage to simulate a non-diagonal (and more interesting) interaction.

6.4.3 Magnus Gadget: What if?

The strength of the Magnus Gadget comes when one can control which couplings gets mediated through the action of commutators. What QuEra is missing in order to have such control is local on-site potentials. If we had that, we could make the interaction:

$$H(t) = u(t)Y_m + \sum_{j>i} V_{ij}N_i^z N_j^z + \left(\sum_i V_{im}N_i^z \right) Z_m$$

The commutators are a lot easier to keep track of in the combinatorical nightmare that is the Magnus expansion, since they only act on the ancilla qubit m . Every term commutes with the Rydberg interaction between the target qubits, so these terms just get factored out of the gadget. The expansion will thus look like:

$$\begin{aligned} \Omega_1 &\in \text{span} \left(Y_m, \sum_i V_{im}N_i Z_m, \sum_{j>i} V_{ij}N_i^z N_j^z \right) \\ \Omega_2 &\in \text{span} \left(\sum_i V_{im}N_i^z X_m \right) \\ \Omega_3 &\in \text{span} \left(\sum_i V_{im}N_i^z Z_m, \left(\sum_i V_{im}N_i^z \right)^2 Y_m \right) \end{aligned}$$

By going to higher orders in the Magnus expansion, we will get higher-order interactions.

As an example, imagine we had three qubits with an ancilla qubit somewhere in the middle between them. If we could apply a time dependent pulse with the property that 1-, 2- and 3-local terms cancel, we could simulate the target Hamiltonian that is the sum of the Magnus interaction and the inherent Rydberg interaction between the target qubits:

$$H_{\text{target}} = N_1^z N_2^z N_3^z (B^x X_m + B^z Z_m) + \frac{t}{\theta(t)} (V_{12}N_1^z N_2^z + V_{13}N_1^z N_2^z + V_{23}N_2^z N_3^z)$$

With renormalized time $\theta(t)$. By for instance choosing the atoms to form an equidistant triangle with the ancilla bit in the middle, we produce the 3-local Hamiltonian above, with interaction strengths $V_{12} = V_{13} = V_{23} = \frac{1}{27}V_{1m} = \frac{1}{27}V_{2m} = \frac{1}{27}V_{3m}$ since the potential scales like $\frac{1}{r^6}$. Hopefully in such a scenario, we would have $27 \cdot \theta(t) \gg t$, for all times, such that the last 2-local terms have marginally smaller weight than the 4-local term, which is the interaction we would mainly like to simulate.

Notice that this in no way was a formal proof of the success of the construction: We assumed that

there exists pulses such that the 1-, 2- and 3-local terms in the Magnus expansion disappears and that the Magnus gadget construction produces the desired 4-local interaction from there. We furthermore had a hope that $\theta(t) \gg \frac{t}{27}$ for all t in order for the construction to be close to the desired "bare" target Hamiltonian but this is not something we have any control over in the gadget.

Hopefully, we could make the same construction with more atoms. By putting higher order conditions on our pulses, we might be able to simulate terms of higher locality without unwanted counter terms, but this toy-heuristic paves the way for how one could attempt this in general.

6.4.4 Cubitt-universality: What if?

Cubitt et al. found that they had simulationwise universality from the class of Hamiltonians:

$$H = \sum_{i,j} \alpha_{ij} A_{ij} + \sum_k \beta_k Z_k + \gamma_k X_k \quad (10)$$

For $\alpha_{ij}, \beta_k, \gamma_k \in \mathbb{R}$ and where $A_{ij} \in \{Z_i Z_j, X_i Z_j, Z_i X_j, X_i X_j\}$. Thus, if the QuEra Hardware can produce all such interactions then it can simulate any Hamiltonian in the framework given by Cubitt et al. The on-site Z 's and X 's come easy on the QuEra-machine given that the machine upgrades to local on-site interactions but the question is if one can produce an arbitrary sum of the four 2-local interactions. It's obvious that one can make the ZZ -interaction for positive α_{ij} but it remains to be seen how one can do it for negative coefficients. It is also less obvious that one can make the other interactions, since only the ZZ -Hamiltonian is native in the QuEra framework.

In further work, it has actually been characterized that any family of Hamiltonians that is non-2SLD acting on qubits with a connectivity graph of a 2D square lattice is universal [27]. Being non-2SLD means that there doesn't exist a unitary $U \in \text{SU}(2)$, such that any Hamiltonian in the family has the property:

$$U^{\otimes 2} H_{ij} (U^\dagger)^{\otimes 2} = \alpha_{ij} Z_i Z_j + A_i \otimes \mathbb{1}_j + \mathbb{1}_i \otimes B_i$$

Where A_i and B_i are any 1-local Hamiltonian. This doesn't bode well for the QuEra framework since its constituents exactly have the form as above. The most natural way to overcome this is to utilize the time dependence of the Hamiltonian since this is not accounted for in the Cubitt framework.

No Magnus gadget application we have found above seems like a good fit to get the QuEra Hamiltonian on the form of equation 10. A first attempt to locally do so would be to apply an on-site pulse with a strength so large that the Rydberg potential is negligible, with the following

forms:

$$\begin{aligned}
 H_{-Z_1 Z_2} &= aY_1 \\
 H_{X_1 Z_2} &= \frac{a}{\sqrt{2}}(X_1 + Z_1) = aH_1 \\
 H_{Z_1 X_2} &= \frac{a}{\sqrt{2}}(X_2 + Z_2) = aH_2 \\
 H_{X_1 X_2} &= \frac{a}{\sqrt{2}}(X_1 + Z_1) + \frac{a}{\sqrt{2}}(X_2 + Z_2) = aH_1 + aH_2
 \end{aligned}$$

Where H_i indicates the Hadamard gate on qubit i and a is a large pulse strength. After waiting $t = \frac{\pi}{2a}$ these would transform $\alpha_{12}Z_1Z_2$ into:

$$\begin{aligned}
 \exp(i\pi H_{-Z_1 Z_2})\alpha_{12}Z_1Z_2 \exp(-i\pi H_{-Z_1 Z_2}) &= -\alpha_{12}Z_1Z_2 \\
 \exp(i\pi H_{X_1 Z_2})\alpha_{12}Z_1Z_2 \exp(-i\pi H_{X_1 Z_2}) &= \alpha_{12}X_1Z_2 \\
 \exp(i\pi H_{Z_1 X_2})\alpha_{12}Z_1Z_2 \exp(-i\pi H_{Z_1 X_2}) &= \alpha_{12}Z_1X_2 \\
 \exp(i\pi H_{X_1 X_2})\alpha_{12}Z_1Z_2 \exp(-i\pi H_{X_1 X_2}) &= \alpha_{12}X_1X_2
 \end{aligned}$$

So that the inherent Rydberg Blockade instead respectively would become a $-\alpha_{12}Z_1Z_2$, $\alpha_{12}X_1Z_2$, $\alpha_{12}Z_1X_2$ - or $\alpha_{12}X_1X_2$ -interaction term . Thus, we would locally be able to make either of the four possible A_{ij} -terms with arbitrary constant α_{ij} in front.

The above construction would work by applying local unitaries on the system such that the 2-local Rydberg interaction gets transformed into terms of the like of equation 10. The problem here is that the different terms ZZ , XZ , ZX and ZZ in the sum don't commute, so there doesn't exist a local unitary which can take the sum of operators $\sum_{ij} Z_i Z_j$, which is simultaneously diagonalized and transform them into the sum $\sum_{ij} A_{ij}$, which can't be simultaneously diagonalized. It is unclear whether it is possible to create such interactions via general unitary transformations of higher locality produced by time-dependent Hamiltonians and thus it is an open question how well the QuEra computer can simulate Hamiltonians in the Cubitt Framework.

7 Conclusion

In conclusion, this master’s thesis offers a comprehensive overview of notions of analogue Hamiltonian simulation and their diverse applications. The thesis begins by introducing analogue Hamiltonian simulation and explores different notions of universality within the context of simulability. It presents examples of known gadgets from the literature, such as the Perturbative and Logical gadgets, which approximate target Hamiltonians of high locality by utilizing the low-energy subspace of a simulator Hamiltonian of lower locality.

Regarding the Perturbative gadget, the thesis not only discusses archetypal examples found in the literature such as the 3-to-2-gadget and subdivision gadget, but also introduces novel perturbative constructions developed by the author. These include the geometric-series-gadget and the direct- k -local gadget, accompanied by numerical demonstrations of their effectiveness. In the case of Logical gadgets, the thesis explores the established AND-gadget, and introduces novel examples like the chain-gadget and the SWAP-gadget.

Shifting the focus to a third type of gadget, the thesis introduces a novel construction by the author, known as the “Magnus gadget”. This construction offers a different approach by characterizing the solution to the time-dependent Schrödinger equation, enabling time-evolution equivalent to that of a time-independent target Hamiltonian with greater locality. The thesis provides heuristics and toy-examples that demonstrate the successful characterization of target Hamiltonians using this method. The strength of the Magnus gadget lies in its ability to operate without forcing the simulator Hamiltonian into its low-energy subspace. However, the method introduces parameters that must be calculated as a truncated Magnus expansion or numerically, and the method solely works heuristically.

After introducing several gadgets, the thesis engages in a discussion on key topics related to their capabilities and limitations. It investigates the connectivities under which different gadgets can simulate a Toffoli-gate and the precision with which they can achieve this simulation. Furthermore, the thesis explores potential approaches for implementing the promise of operating within the low-energy subspace of a simulator Hamiltonian, including coupling the system to a bath, quantum annealing, and verification protocols for examining the validity of the promise. To top it off, it gives a brief summary of the strengths and weaknesses of each gadget.

The thesis concludes by applying the discussed gadgets to the QuEra hardware platform, an analogue Hamiltonian quantum simulator. It demonstrates that a version of the Perturbative gadget can successfully simulate 3-local interactions, with the 3-local part asymptotically approaching zero as the error decreases. Additionally, a version of the Logical gadget referred to as a toy-gadget accurately simulates an almost bare 3-local interaction with zero error in the low-energy regime. The thesis further shows that the Magnus Gadget can redirect the native, time-independent two-local interaction from a ZZ -interaction to another, such as an XX -interaction.

To expand on these findings, the thesis speculates on the possibilities of QuEra simulation

scenarios where on-site control is local instead of global. It suggests that a Toffoli-gate can be applied, at least approximately via the Logical gadget. Additionally, the thesis explores the potential for the QuEra framework to serve as a universal simulator within the Cubitt Framework. While it establishes local implementation between two atoms, it encounters limitations in creating interactions beyond ones that are 2SLD when more atoms are involved, thus not proving universality.

In summary, this thesis offers a contribution to the field of analogue Hamiltonian simulation, providing researchers with a resource for further study and development. The work of the thesis provides valuable insights and a comprehensive overview of the topic. Researchers can leverage the findings and methodologies discussed in this thesis as a stepping stone for future advancements in analogue Hamiltonian simulation.

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References

- [1] AHARONOV, D. A Simple Proof that Toffoli and Hadamard are Quantum Universal, Jan. 2003. arXiv:quant-ph/0301040.
- [2] AVRON, J. E., AND ELGART, A. Adiabatic Theorem without a Gap Condition. *Communications in Mathematical Physics* 203, 2 (June 1999), 445–463.
- [3] BENIOFF, P. The computer as a physical system: A microscopic quantum mechanical Hamiltonian model of computers as represented by Turing machines. *Journal of Statistical Physics* 22, 5 (May 1980), 563–591.
- [4] BIAMONTE, J. D. Non-perturbative k-body to two-body commuting conversion Hamiltonians and embedding problem instances into Ising spins. *Physical Review A* 77, 5 (May 2008), 052331. arXiv:0801.3800 [quant-ph].
- [5] BLANES, S., CASAS, F., OTEO, J. A., AND ROS, J. The Magnus expansion and some of its applications. *Physics Reports* 470, 5-6 (Jan. 2009), 151–238. arXiv:0810.5488 [math-ph].
- [6] CAO, Y., BABBUSH, R., BIAMONTE, J., AND KAIS, S. Experimentally Realizable Hamiltonian Gadgets.
- [7] CASAS, F. Sufficient conditions for the convergence of the Magnus expansion. *Journal of Physics A: Mathematical and Theoretical* 40, 50 (Dec. 2007), 15001–15017. arXiv:0711.2381 [math].
- [8] CASAS, F. C. F. The Magnus expansion and its physical applications.
- [9] CIPRA, B. A. The ising model is np-complete.
- [10] CUBITT, T., MONTANARO, A., AND PIDDOCK, S. Universal Quantum Hamiltonians. *Proceedings of the National Academy of Sciences* 115, 38 (Sept. 2018), 9497–9502. arXiv:1701.05182 [quant-ph].
- [11] DEÇORDI, G. L., AND VIDIELLA-BARRANCO, A. Two coupled qubits interacting with a thermal bath: A comparative study of different models. *Optics Communications* 387 (Mar. 2017), 366–376. arXiv:1406.0528 [cond-mat, physics:physics, physics:quant-ph].
- [12] FEYNMAN, R. P. Simulating physics with computers. *International Journal of Theoretical Physics* 21, 6 (June 1982), 467–488.
- [13] GALLIER, J. The Schur Complement and Symmetric Positive Semidefinite (and Definite) Matrices.
- [14] GRIFFITHS, D. *Introduction of Quantum Mechanics*. Prentice Hall, Inc., 1995.

- [15] HOUSE, M. E. The Physics of Computation Conference, Mar. 2018.
- [16] ITANO, W. M. Perspectives on the quantum Zeno paradox. *Journal of Physics: Conference Series* 196, 1 (Nov. 2009), 012018.
- [17] JONATHAN, D., AND PLENIO, M. B. Entanglement-assisted local manipulation of pure quantum states. *Physical Review Letters* 83, 17 (Oct. 1999), 3566–3569. arXiv:quant-ph/9905071.
- [18] KEMPE, J., KITAEV, A., AND REGEV, O. The Complexity of the Local Hamiltonian Problem, Oct. 2005. arXiv:quant-ph/0406180.
- [19] KNORR, A. Quera - quantum computing with neutral atoms:, nov 2022. PIRSA:22110095 see, <https://pirsa.org>.
- [20] MIZEL, A., LIDAR, D., AND MITCHELL, M. Simple Proof of Equivalence between Adiabatic Quantum Computation and the Circuit Model. *Physical review letters* 99 (Sept. 2007), 070502.
- [21] NATION, P. D., JOHANSSON, J. R., PITCHFORD, A. J. G., GRANADE, C., GRIMSMO, A. L., SHAMMAH, N., AHMED, S., LAMBERT, N., LI, B., LISHMAN, J., CROSS, S., AND GIGUÈRE, E. QuTiP: Quantum Toolbox in Python.
- [22] NGUYEN, M.-T., LIU, J.-G., WURTZ, J., LUKIN, M. D., WANG, S.-T., AND PICHLER, H. Quantum optimization with arbitrary connectivity using Rydberg atom arrays. *PRX Quantum* 4, 1 (Feb. 2023), 010316. arXiv:2209.03965 [cond-mat, physics:physics, physics:quant-ph].
- [23] NISAN, N., AND SCHOCKEN, S. *The Elements of Computing Systems: Building a Modern Computer from First Principles (History of Computing S.)*. The MIT Press, 2008.
- [24] OLIVEIRA, R., AND TERHAL, B. M. The complexity of quantum spin systems on a two-dimensional square lattice, June 2008. arXiv:quant-ph/0504050.
- [25] RIVAS, A., AND HUELGA, S. F. *Open Quantum Systems. An Introduction*. 2012. arXiv:1104.5242 [cond-mat, physics:math-ph, physics:physics, physics:quant-ph].
- [26] SHENDE, V. V., AND MARKOV, I. L. On the CNOT-cost of TOFFOLI gates, Mar. 2008. arXiv:0803.2316 [quant-ph].
- [27] ZHOU, L., AND AHARONOV, D. Strongly Universal Hamiltonian Simulators, Feb. 2021. arXiv:2102.02991 [cond-mat, physics:quant-ph].