Time Simulation of an Anisotropic Heisenberg Chain in a Superconducting Quantum Processor

Undergraduate Thesis

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Contents

Abstract

This work proposes a digital quantum algorithm for simulating time evolution of a completely anisotropic Heisenberg Hamiltonian on an arbitrary lattice. Experiments were performed on IBM Q devices, and fidelities greater than 80% were obtained for spin chains with up to 4 lattice sites. Moreover, the gate count is significantly improved over similar algorithms, and by the nature of the gates used, transpilation to IBM Q devices is quite cost effective. As an interesting application, the algorithm is used to construct a quantum node for producing thermal states of a magnetic lattice whose dynamics is governed by a Heisenberg-like Hamiltonian.

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Chapter 1

Introduction

Quantum Computing has become a reality now that the field is entering the so called NISQ (Noisy Intermediate Quantum) era. The digital quantum circuit model is one of the most extended and discussed. It is based upon the concept of qubit, which is an abstract two-level quantum system. By profiting linear superposition and entanglement of many-qubit systems, quantum algorithms are thought to be more resource-efficient than standard classical algorithms in areas like machine learning and mathematical finance. The present work studies a more fundamental, yet quite versatile, application of quantum computation: simulation of quantum physical systems. This perspective was introduced in 1982 by Richard Feynman [7]. He suggested that using a quantum system to simulate another can reduce the exponential overhead that occurs by incrementing the number of components.

In particular, this work is concerned with the task of devising a quantum time simulator capable of performing evolution of parametric Heisenberg anisotropic models. A digital quantum algorithm for such tasks, based on Trotter decomposition, is devised using Qiskit SDK. At the moment of presentation of this dissertation, Las Heras et. al. [8] and Y. Salathé et. al. [12] have proposed simple digital quantum algorithms for simulating time evolution of small Heisenberg systems. The circuits employed by those groups, however, where specifically optimized for superconducting chips whose architecture is not publicly available. This work extends those insights and adapts them to the architecture available publicly by IBM Quantum through Qiskit SDK. Furthermore, effects of noise in Trotter-based simulation algorithms are discussed and simulated, as well as the capabilities of quantum time evolution for computing ground state properties via quantum annihilation.

Since 2021, Qiskit has extended their circuit library to include simulation of multi-qubit Hamiltonians using Suzuki-Trotter schemes. Most of those schemes are based upon a direct partition of the target hamiltonian in a Pauli-product basis. In the present work, a slightly more sophisticated approach, based on the nature of the specific Heisenberg model Hamiltonian is shown to produce lower circuit depth and a shorter execution time, for given accuracy. Furthermore, since fault-tolerant quantum computing is still a work in progress, variational approaches to quantum time simulation are discussed and implemented using Qiskit SDK.

This dissertation is structured in 4 chapters. After a review of the main concepts of quantum computing (chapter 2), the fundamentals of quantum time simulation are revised on chapter 3. Here, as an illustration, the circuits proposed by Las Heras et. al. [8] and Y. Salathé et. al. [12] are simulated using Qiskit SDK. On chapter 4, these circuits are revisited and optimized in order to produce lower circuit depths, and potentially better state fidelity. Experimental and theoretical state fidelities produced by the algorithm are discussed in this chapter too. Moreover, the influence of noisy channels in the evolution schemes is discussed using models from Qiskit Ignis. Finally, on chapter 5, due to the limitations of current quantum devices, a variational quantum time evolution algorithm is introduced and implemented.

Chapter 2

Quantum Computing

This chapter introduces the elements of quantum computing. First, the qubit as a two-level system and a quantum register as a *multi-qubit* system are presented. Then, unitary operations on a quantum register's Hilbert space are introduced as the quantum analogue of digital logic gates. This leads to the question about how to represent any unitary operator on a quantum register using quantum gates. Thereby introducing the concept of universal basis gates sets. Finally, a digression about the capabilities of quantum computing for the general theory of computations is presented.

2.1 Quantum circuit model elements

Nowadays, it is familiar to understand information processing tasks in terms of *bits*. A bit is a binary variable that can be said to have either of two states on a set (commonly denoted by 0, 1). As a result, a bit is nothing more than a variable s whose value is in the set $\{0,1\}$. In modern computers, such an entity can be encoded physically by means of electric current or voltage. Most operations that can act upon a bit are mappings from one of the possible state values to the other. These corresponds to two fundamental operations: the NOT gate, which flips the bit value, or the IDENTITY gate, whose action is actually inaction.

In contrast, a quantum bit or *qubit*, corresponds physically to a two-level quantum system, whose Hilbert space can be spanned by a *computational basis set* $\{|0\rangle, |1\rangle\}$. It is reasonable to assume that this basis set is orthonormal

$$\langle s | s' \rangle = \delta_{ss'} \text{ for } s, s' \in \{0,1\} \tag{2.1}$$

The canonical representation of a qubit is as a vector in the *Bloch sphere*. This representation maps a generic qubit superposition state

$$\cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle \tag{2.2}$$

$$\theta, \phi \in \mathscr{R} \tag{2.3}$$

To a vector on the unitary 3-sphere

$$\hat{\mathbf{n}} = \sin(\theta)\cos(\phi)\hat{\mathbf{x}} + \sin(\theta)\sin(\phi)\hat{\mathbf{y}} + \cos(\theta)\hat{\mathbf{z}} \tag{2.4}$$

In addition to the computational basis, other important states are the *sign basis*

$$|+\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle \tag{2.5}$$

$$|-\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle \tag{2.6}$$

And the *y basis*

$$|+\mathrm{i}\rangle = \frac{1}{\sqrt{2}}|0\rangle + \mathrm{i}\frac{1}{\sqrt{2}}|1\rangle \tag{2.7}$$

$$|-\mathrm{i}\rangle = \frac{1}{\sqrt{2}}|0\rangle - \mathrm{i}\frac{1}{\sqrt{2}}|1\rangle \tag{2.8}$$

Those states actually lie in the poles of the Bloch sphere, and each pair constitutes a basis for a qubit's Hilbert space that has interesting properties regarding measurement.

In contrast to classical bits, a quantum bit can be transformed by an infinite number of operations, corresponding to all possible operators defined on its Hilbert space. Of those, two are of huge importance in quantum computing: unitary operators and measurement operators. Unitary operations are used mainly to process quantum information and perform a computation. These are commonly known as *quantum gates*. The fundamental quantum gates are the Pauli operators

$$\hat{X} = |+\rangle\langle+| - |-\rangle\langle-| \tag{2.9}$$

$$\hat{Y} = |+\mathrm{i}\rangle\langle+\mathrm{i}| - |-\mathrm{i}\rangle\langle-\mathrm{i}| \tag{2.10}$$

$$\hat{Z} = |0\rangle\langle 0| - |1\rangle\langle 1| \tag{2.11}$$

For a single qubit, it is known that any unitary operation can be represented as rotation operator of the form

$$\hat{R}_{\hat{n},\theta} = \cos\left(\frac{\theta}{2}\right) - \mathrm{i}\sin\left(\frac{\theta}{2}\right)\hat{n}\cdot\sigma \tag{2.12}$$

$$\hat{n}\cdot\sigma = n_x\hat{X} + n_y\hat{Y} + n_z\hat{Z} \tag{2.13}$$

$$||\hat{n}||^2 = 1 \tag{2.14}$$

In the Bloch sphere representation, quantum gates, therefore, correspond to rotations of the quantum state's associated vector (eq. 2.4). A quite important rotation is the so called *Hadamard gate*, whose representation in the computational basis is

$$\hat{H} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{2.15}$$

These rotations allow computations, but the actual process of reading the outcome of an algorithm implies measurement. In current digital quantum computing implementations, measurement operators are projectors onto the computational basis

$$\hat{P}_0 = |0\rangle\langle 0| \tag{2.16}$$

$$\hat{P}_1 = |1\rangle\langle 1| \tag{2.17}$$

These operators allow measurement of the expected value of $\hat{Z}$ operator. By performing rotations to the sign and y basis, it is possible to measure expected values of $\hat{X}$ and $\hat{Y}$, respectively. Since Pauli operators span the space of qubit operators, any qubit observable can be measured by applying suitable rotations and forming linear combinations of expected values of Pauli operators.

2.1.1 Quantum registers and multi-qubit gates

In general, more than one qubit is needed to perform meaningful computations. A system of several qubits is called *quantum register*. A quantum register's Hilbert space is nothing more than the tensor product space of each of its constituent qubits. Thus, a N-qubit register has a 2^N-dimensional Hilbert space. A basis for this space is built by all possible tensor products of computational basis states for each qubit. This would be the *computational basis* of the register. A member of this set may be denoted by

$$|s_{N-1}s_{N-2}\cdots s_0\rangle = |s_{N-1}\rangle \otimes |s_{N-2}\rangle \otimes \cdots \otimes |s_0\rangle \tag{2.18}$$

$$s_{N-1}, s_{N-2}, \ldots, s_0 \in \{0,1\} \tag{2.19}$$

There may be other basis of interest in quantum computing. For instance, with $N = 2$, the so called *Bell basis*,

$$\left|\Phi^{+}\right\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \tag{2.20}$$

$$|\Phi^{-}\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \tag{2.21}$$

$$\left|\Psi^{+}\right\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \tag{2.22}$$

$$|\Psi^{=}\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle) \tag{2.23}$$

is of capital importance in quantum information theory and quantum communications. It will also prove to be important in this work. Much like single-qubit gates, register gates or multi-qubit gates correspond to unitary operators defined on the register's Hilbert space. An important multi-qubit gate, defined by its action on two qubits is CNOT

$$\mathrm{CNOT}\left|\psi\right\rangle_t \otimes |1\rangle_c = \left(\hat{X}\left|\psi\right\rangle_t\right) \otimes |0\rangle_c \tag{2.24}$$

$$\mathrm{CNOT}\left|\psi\right\rangle_t \otimes |0\rangle_c = \left|\psi\right\rangle_t \otimes |0\rangle_c \tag{2.25}$$

Where the subscript t denotes the *target* qubit, and the subscript c, the control qubit. Hence, CNOT corresponds to a controlled-$\hat{X}$ operation. This gate can entangle separable two-qubit states. This is of vital importance for universal quantum computing, and can be readily seen from the definition.

2.1.2 Circuit representation

This model of computation can be represented graphically by a *circuit*, in which every wire represents a quantum bit, and a gate corresponds to a unitary operator acting on the register's Hilbert space (possibly a Hilbert subspace). For instance, an algorithm for producing a Bell basis state can be represented as in fig. 2.1

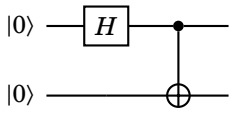

Figure 2.1: Simple algorithm for producing Bell state $\left|\Phi^{+}\right\rangle$

In this circuit representation, the algorithm depicted consists on an application of a hadamard operator to a control qubit, followed by a CNOT operation, to a two qubit register on state $|00\rangle$. In general, quantum gates are represented by boxes, labeled properly by the operation that represent. These boxes cover the subspace over which the corresponding quantum operator acts. For instance, in the case of the algorithm depicted on fig. 2.1, the Hadamard gate acts on a single-qubit subspace, where the CNOT gate acts on the whole two-qubit register's space. Operations are executed from left to right in a quantum algorithm.

2.2 Universal quantum computing

As was stated before, all quantum gates correspond to unitary operations (or measurements), acting on a quantum register. It is desirable to find a set of elementary quantum gates, that act on a small number of qubits, that can generate all possible unitary operations on an N-qubit register. This is the question of universal quantum computing. It can be shown that CNOT and the set of single-qubit unitary operations are enough for producing all possible N-qubit register gates [11]. For instance, it is possible to perform the three-qubit *Controlled CNOT* operation

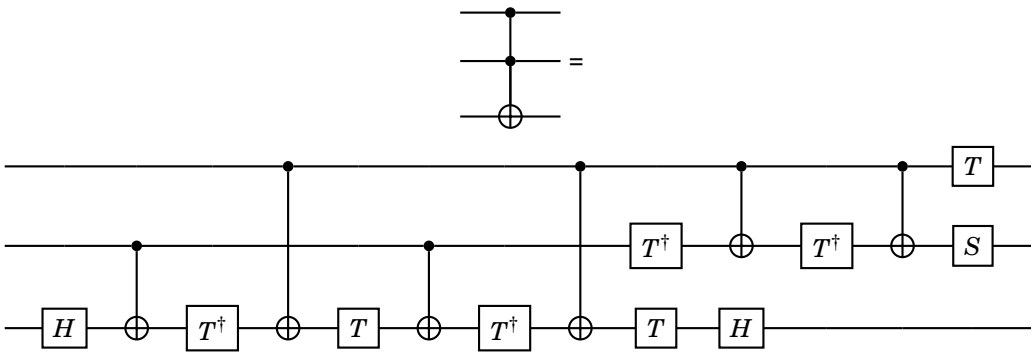

Figure 2.2: Representation of CCNOT (L. H. S.) gate in terms of single-qubit rotations and CNOT (R. H. S.), according to [11]. Here $\hat{S} = \sqrt{\hat{Z}}$ and $\hat{T} = \sqrt{\hat{S}}$.

$$\mathrm{CCNOT}\left|\psi\right\rangle \otimes \left|s_t\right\rangle \otimes \left|s_t'\right\rangle = \left(\hat{X}^{s_t s_t'}\left|\psi\right\rangle\right) \otimes \left|s_t\right\rangle \otimes \left|s_t'\right\rangle \tag{2.26}$$

$$s_t, s_t' \in \{0,1\} \tag{2.27}$$

by following algorithm on figure 2.2. In general, however, performing arbitrary single-qubit rotations by hardware operations is impractical. This would require a huge control on the physical qubits that is not yet available for all possible architectures [11]. As a result, most quantum processors available today use a limited set of single-qubit rotations for *approximating* arbitrary rotations.

A commonly used universal set is $\{\hat{H}, \hat{S} = \sqrt{\hat{Z}}, \hat{T} = \sqrt{\hat{S}}\}$. With this set, it is possible to approximate any single qubit rotation to an arbitrary precision, but not exactly, using a finite number of operations. In contrast, IBM Quantum devices use a basis set $\{\hat{S}_x = \sqrt{\hat{X}}, \hat{X}, \hat{R}_{z,\phi}\}$, which can reproduce any single-qubit rotation exactly. As an example, the Hadamard gate can be decomposed as follows

$$\hat{H} = \hat{R}_{z,\pi/2}\hat{S}_x\hat{R}_{z,\pi/2} \tag{2.28}$$

As may be inferred from the two examples above, emulating arbitrary N-qubit-register operators can cause some computational overhead, that is an increase in the number of elementary operations required to reproduce a quantum computation. Usually, the basis set depends on the architecture of a quantum processor, and thus, due to current limitations of available hardware, it is important to design a quantum algorithm so that the operations involved can be optimally represented by the universal set associated to the device on which it is expected to be implemented.

2.3 Quantum computational advantage

It is expected that quantum computing paradigms challenge the strong Church-Turing thesis, which claims that the ultimate reference for computational complexity is the probabilistic Turing Machine Model [11, 4]. In principle, a quantum processor could solve problems that are thought to be hard for probabilistic Turing Machines. Such problems include simulation of chemical systems [10, 5], and multi-particle quantum systems in general [11, 1, 6]. Regarding the quantum circuit model of computation, this usually means that the total gate count of a circuit that implements an algorithm that solves a hard problem is bounded asymptotically by a polynomial function in the size of the input [11, 4]. In general, however, a more accurate measurement of the complexity of a quantum algorithm is the *circuit depth*, which measures the maximum number of operations a qubit has to undergo to complete a computation. One of the goals of this work is to show that it is possible to simulate arbitrarily large spin systems efficiently using quantum digital algorithms, something impossible with the standard methods of computational quantum physics.

Chapter 3

Quantum Time Simulation

An introduction to quantum time simulation, as opposed to *classical* time simulation of quantum systems is presented on section 3.1. After that, a generic framework for approximate quantum time evolution is presented on section 3.2 Finally, on section 3.3, quantum digital simulations of one-dimensional Hubbard models, carried out by Las Heras et. al. [8] and Barends et. al. [2], are discussed as immediate predecessors of this works.

3.1 Quantum Time Simulation v. Classical Time Simulation

At the heart of simulation of quantum physical systems is solving Schrödinger's equation of motion [3, 11]:

$$\mathrm{i}\frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi\rangle \tag{3.1}$$

Where $\hat{H}$ is the Hamiltonian that defines the interaction between the system's components, and perhaps its environment. In position representation, A one-dimensional system of spinless particles can be simulated by solving the equation

$$\mathrm{i}\frac{\partial|\psi\rangle}{\partial t} = \left[\sum_{i=1}^{n}\frac{\hat{P}_i^2}{2m_i} + \hat{V}(x_1,x_2,\ldots,x_n)\right]|\psi\rangle \tag{3.2}$$

Supposed $|\psi\rangle$ represents an n-particle system state. Hence, a single particle dynamics can be determined by solving the equation

$$\mathrm{i}\frac{\partial|\psi\rangle}{\partial t} = \left[\frac{\hat{P}^2}{2m} + \hat{V}(x)\right]|\psi\rangle \tag{3.3}$$

A classical algorithm may use a fine discretization of position basis, in some spatial region $S = [0,L]$, with a basis of N statevectors and a discretization step $\Delta x = L/(N-1)$. Such that

$$|x\rangle \text{ for } x \in S \rightarrow |k\Delta x\rangle \text{ for } k = 0,1,\ldots,N-1 \tag{3.4}$$

This scheme leads to a representation of any single particle position state as a linear combination of discrete statevectors

$$|\psi(t)\rangle = \sum_{k=0}^{N-1} a_k(t)|k\Delta x\rangle \tag{3.5}$$

Momentum operator could be approximated using finite difference formulas, thus leading to a system of coupled differential equation on the expansion coefficients a_k

$$\mathrm{i}\frac{\partial a_k}{\partial t} = \sum_{l=0}^{N} H_{kl}a_l \tag{3.6}$$

Solution of equation 3.6, given $a_k(0)$, would yield a complete knowledge of the particle's dynamics at any time. Typically, this would require diagonalization of the Hamiltonian matrix, H_{kl}. There

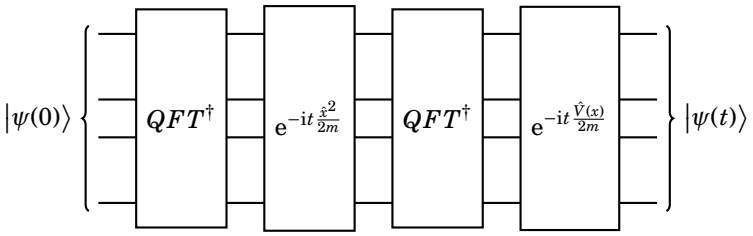

Figure 3.1: Time evolution slice for a single particle state on a digital quantum computer. This step should be repeated several times, with a time step dt, which depends upon the desired error bound and spatial discretization.

are more efficient approaches than this, of course. For instance, Numerov integration. However, the goal of this example is to introduce quantum time simulation on a digital quantum computer as smoothly as possible.

Time simulation on a digital quantum computer could be carried out in a very different way [4, 11]. A schematic is presented on figure 3.1. Pretty much in the same way as in the naïve example discussed before, position basis may be discretized. Nevertheless, this time the coefficients would be encoded directly as the amplitudes of the statevector of an n-qubit computer. It is readily seen that to achieve a discretization with N system statevectors, only $\mathcal{O}(\log N)$ qubits are needed. Although not very significant for a single particle, this illustrates that quantum computers have inherent exponential advantage over classical computers in terms of space resources. Instead of diagonalizing the Hamiltonian, digital quantum time simulation relies on the direct solution

$$|\psi(t)\rangle = \exp\left(-i\int_{t_0}^{t}\hat{H}(t)dt\right)|\psi(0)\rangle \tag{3.7}$$

Which for time-independent Hamiltonians reduces to

$$|\psi(t)\rangle = e^{-i(t-t_0)\hat{H}}|\psi(0)\rangle \tag{3.8}$$

In the naïve example considered until now, time evolution with a digital quantum computer amounts to computing unitary operator ($t_0 = 0$)

$$\hat{U}(t) = e^{-it\frac{\hat{p}^2}{2m}}e^{-it\hat{V}(x)} + \mathcal{O}(t^2) \tag{3.9}$$

Using Baker-Haussdorf formulae, or a Suzuki-Trotter scheme of higher order, better expressions for the time evolution operator of the system may be obtained. Notice that operator

$$\hat{U}_P = e^{-it\frac{\hat{p}^2}{2m}}$$

Is efficiently computable, using the Quantum Fourier Transform Algorithm:

$$\hat{U}_P = QFT\, e^{-it\frac{\hat{x}^2}{2m}} QFT^\dagger$$

Therefore, if operator

$$\hat{U}_V = e^{-it\hat{V}(x)}$$

Is efficiently computable, time simulation on a quantum computer might be more resource-friendly, both in terms of space and time, than common simulation using classical computers. Only theoretical constraints are error bounds for a given simulation time interval. Given simulation time and error bound, a time slice dt is fixed, and thus repeated application of operator $\hat{U}(dt)$ evolves a single particle state from some initial state $|\psi(0)\rangle$, to state $|\psi(t)\rangle$.

In summary, rather than using physical bits to encode the expansion coefficients of a particle's state, like on a classical computer, a quantum algorithm relies on the nature of qubits to encode directly such a state. This leads to an exponential reduction in the space complexity of the problem. Furthermore, multi-qubit gates can be used to implement unitary evolution, without the explicit need of matrix diagonalization. Thus leading to a potentially faster evolution simulation. For a

simple system like this, codification of the information of all expansion coefficients would require at least $2N$ reals parameters. Furthermore, diagonalization of the Hamiltonian matrix, H_{kl}, would require $\mathcal{O}(N^2)$ computational steps. As a result, the simulation advantage posed by quantum computation seems unnecessary. Also, there are numerous efficient classical algorithms for solving Schrodinger's time dependent equation, such as Numerov or Runge-Kutta integration. However, this example illustrates the difference between classical simulation and quantum simulation using a digital quantum computer, and some of the possible advantages of quantum time simulation using the former type of information processors.

For a one-dimensional system of several particles, equation 3.6 can be generalized easily. However, the number of coefficients required to describe a statevector in a discrete basis would grow exponentially with the number of particles. As well as matrix Hamiltonian size. As a result, simulation of time dynamics on a classical computer results impractical. Therefore, quantum time simulation of multi-particle systems is an application to which digital quantum computers may represent a practical advantage. In the following sections, common techniques for quantum time simulation in digital computers are presented. In particular, simple approximation formulas are discussed and compared.

3.2 Common Approximation Schemes for Unitary Evolution

Consider a system of N components, whose Hamiltonian can be expressed as a sum of local Hamiltonians (i. e. that model interaction between at most C components) [11, 9]

$$\hat{H} = \sum_{k=1}^{L} \hat{H}_k \tag{3.10}$$

Where L is some polynomial on the number of system components. In general, $[\hat{H}_i, \hat{H}_j] \neq 0$, and thus

$$\mathrm{e}^{-\mathrm{i}\hat{H}t} \neq \prod_{k=1}^{L} \mathrm{e}^{-\mathrm{i}\hat{H}_k t} \tag{3.11}$$

Many systems are described by local interactions, for instance, electrons in a solid material or magnetic moments in a lattice. In several cases, local interaction Hamiltonians are non-commuting, and thus approximation methods are necessary for performing time evolution. In this section, schemes for approximating unitary evolution of a quantum system are discussed.

3.2.1 Trotter Formulas

Consider operators $\hat{H}_1$, $\hat{H}_2$, with $[\hat{H}_1, \hat{H}_2] \neq 0$. By definition

$$\mathrm{e}^{-\mathrm{i}\hat{H}_1 t} = \sum_{m=0}^{\infty} \frac{(-\mathrm{i}t)^m}{m!} \hat{H}_1^m \tag{3.12}$$

$$\mathrm{e}^{-\mathrm{i}\hat{H}_2 t} = \sum_{l=0}^{\infty} \frac{(-\mathrm{i}t)^l}{l!} \hat{H}_2^l \tag{3.13}$$

It is readily shown that

$$\mathrm{e}^{-\mathrm{i}\hat{H}_1 t}\mathrm{e}^{-\mathrm{i}\hat{H}_2 t} = \sum_{k=0}^{\infty} \frac{(-\mathrm{i}t)^k}{k!} \left[\sum_{m=0}^{k} \binom{k}{m} \hat{H}_1^m \hat{H}_2^{k-m} \right] \tag{3.14}$$

Fon non-commuting operators, it is so that

$$\sum_{m=0}^{k} \binom{k}{m} \hat{H}_1^m \hat{H}_2^{k-m} = (\hat{H}_1 + \hat{H}_2)^k + f_k(\hat{H}_1, \hat{H}_2) \tag{3.15}$$

Where $f_k(\hat{H}_1, \hat{H}_2)$ is a function of the commutator of the operators. Since $f_1(\hat{H}_1, \hat{H}_2) = 0$, it is so that

$$\mathrm{e}^{-\mathrm{i}\hat{H}_1 t}\mathrm{e}^{-\mathrm{i}\hat{H}_2 t} = \mathrm{e}^{-\mathrm{i}(\hat{H}_1 + \hat{H}_2)t} + \mathcal{O}(t^2) \tag{3.16}$$

If $|t| \ll 1$, the product of the exponential operators estimate the evolution operator with an error $\mathcal{O}(t^2)$. In the general case, it must be noted that

$$e^{-i\sum_{k=0}^{L}\hat{H}_k t} = \hat{1} + (-it)\sum_{k=0}^{L}\hat{H}_k + \frac{(-it)^2}{2}\left[\sum_{k=0}^{L}\hat{H}_k^2 + 2\sum_{j>k}\hat{H}_k\hat{H}_j\right] + \mathcal{O}(t^3) \tag{3.17}$$

In consequence, a unitary evolution operator with local interactions may be approximated, to quadratic order, by the exponential product

$$e^{-i\sum_{k=0}^{L}\hat{H}_k t} = \prod_{k=1}^{L} e^{-i\hat{H}_k t} + \mathcal{O}(t^2) \tag{3.18}$$

In some instances, quadratic approximations may be enough. In his seminal paper, Lloyd presents this quadratic approximation for simulation of quantum systems with local interaction [9]. Also, Las Heras et. al. simulate a Hubbard Hamiltonian with up to 4 fermionic modes using second order approximations to unitary evolution [2, 8]. However, in following sections, higher-order approximation schemes are discussed, based upon equation 3.17.

3.2.2 Some Cubic Order Schemes

The first cubic order approximation discussed is the so called Baker-Haussdorf formulae [11]. By series expansion, it can be shown that

$$\begin{aligned} e^{-i\hat{H}_1 t}e^{-i\hat{H}_2 t}e^{-i[\hat{H}_1,\hat{H}_2]t^2} =& \hat{1} + (-it)(\hat{H}_1 + \hat{H}_2) \\ &+ \frac{(-it)^2}{2}(\hat{H}_1^2 + \hat{H}_2^2 + \hat{H}_1\hat{H}_2 + \hat{H}_2\hat{H}_1) + \mathcal{O}(t^3) \\ =& e^{-i(\hat{H}_1+\hat{H}_1)t} + \mathcal{O}(t^3) \end{aligned}$$

Although useful in case of operators that constitute a Lie algebra, the formulae above may not be enough in other instances. A more general approximation formulae is

$$e^{-it\sum_{l=0}^{L-1}\hat{H}_l} = \left(\prod_{l=0}^{L-1} e^{-i\hat{H}_l\frac{t}{2}}\right)\left(\prod_{l=L-1}^{0} e^{-i\hat{H}_l\frac{t}{2}}\right) + \mathcal{O}(t^3) \tag{3.19}$$

This can be deduced directly from the identity

$$e^{-i\sum_{l=0}^{2L-1}\hat{K}_l t} = \hat{1} + (-it)\sum_{l=0}^{2L-1}\hat{K}_l + \frac{(-it)^2}{2}\left[\sum_{l=0}^{2L-1}\hat{K}_l^2 + 2\sum_{j>l}\hat{K}_l\hat{K}_j\right] + \mathcal{O}(t^3) \tag{3.20}$$

With the identifications

$$\hat{K}_l = \hat{K}_{2L-1-l} = \frac{\hat{H}_l}{2} \tag{3.21}$$

And the following observations

$$\begin{aligned} \sum_{l=0}^{2L-1}\hat{K}_l^2 &= \frac{1}{2}\sum_{l=0}^{L-1}\hat{H}_l^2 \\ 2\sum_{l'>l}\hat{K}_l\hat{K}_{l'} &= \frac{1}{2}\sum_{l=0}^{L-1}\hat{H}_l^2 + \sum_{l'>l}\left(\hat{H}_l\hat{H}_{l'} + \hat{H}_{l'}\hat{H}_l\right) \\ \left(\sum_{l=0}^{L-1}\hat{H}_l\right)^2 &= \sum_{l=0}^{L-1}\hat{H}_l^2 + \sum_{l'>l}\left(\hat{H}_l\hat{H}_{l'} + \hat{H}_{l'}\hat{H}_l\right) \end{aligned} \tag{3.22}$$

3.2.3 Suzuki - Trotter Scheme

This scheme is a higher order approximation to an evolution operator, that works iteratively on top of the approximation given by equation 3.19. Define [13, 6]

$$\hat{S}_2(\lambda) = \prod_{l=0}^{L-1} e^{\frac{\lambda}{2}\hat{H}_l}\prod_{l=L-1}^{0} e^{\frac{\lambda}{2}\hat{H}_l} \tag{3.23}$$

Then, for $k > 1$, the following recursion relation is defined

$$\hat{S}_{2k}(\lambda) = [\hat{S}_{2k-2}(p_k\lambda)]^2 \hat{S}_{2k-2}((1-4p_k)\lambda)[\hat{S}_{2k-2}(p_k\lambda)]^2 \tag{3.24}$$

Where coefficients p_k are defined as

$$p_k = \frac{1}{4 - 4^{\frac{1}{2k-1}}} \tag{3.25}$$

It has been shown by Suzuki that [13]

$$\mathrm{e}^{-\mathrm{i}t\sum_{l=0}^{L-1}\hat{H}_l} = \hat{S}_{2k}(-\mathrm{i}t) + \mathcal{O}(t^{2k+1}) \tag{3.26}$$

On [6], Barry et. al. show that Suzuki-Trotter schemes can efficiently simulate sparse Hamiltonians, such as the ones considered in this work. As a matter of fact, they have shown that the number of exponentials ($N_{\exp}$) required to simulate time evolution of a system during a time interval $t > 0$, with error bounded by $\epsilon > 0$, is such that

$$N_{\exp} \leq 2L5^{2k}(L\tau)^{1+1/2k}/\epsilon^{1/2k} \tag{3.27}$$

Where $\tau = \left\|\hat{H}\right\| t$, $2k$ is the order of a Suzuki-Trotter iteration, and $\epsilon \leq 1 \leq 2L5^{2k}$. Notice that by choosing a sufficiently high order, a Suzuki-Trotter scheme can emulate time evolution with almost linear complexity in time.

In most cases, simulation of a quantum system by a digital quantum computer requires mapping its Hilbert space to a 2^M-dimensional Hilbert space. In that case, the number of qubits required for simulation would be M. Clearly, all quantum operators in the simulated system's space should be mapped to operators on an M-qubit space, which would then be approximated by a universal set of gates. In the following section, demonstrations of this approach to the study of the Hubbard Model and the Electronic structure problem are introduced.

3.3 Examples of Quantum Time Simulation

On section 3.1, a comparison between classical time simulation and quantum time simulation was introduced. In particular, a scheme for integrating Schrödinger's equation for a n-particle system was proposed. This section introduces examples of simulation of Hamiltonians of the type

$$\hat{H} = \sum_{\langle i,j\rangle} J_{ij}^{(x)}\hat{X}_i\hat{X}_j + J_{ij}^{(Y)}\hat{Y}_i\hat{Y}_j + J_{ij}^{(Z)}\hat{Z}_i\hat{Z}_j + \sum_i H_i^{(X)}\hat{X}_i + H_i^{(Y)}\hat{Y}_i + H_i^{(Z)}\hat{Z}_i \tag{3.28}$$

Defined over an arbitrary spin graph, and considering nearest neighbor interaction. Most of them are related to work from Las Heras et. al. [2, 8] and Y. Salathé [12]. In this section, the importance of simulating this type of systems is discussed. Furthermore, these examples are further generalized in following chapters to simulate any system whose Hamiltonian is of the shape of eq. 3.28, and its limitations are exemplified.

3.3.1 Digital simulation of two-spin models

As a first example, simulation of two-spin models carried out by Y. Salathé et. al. [12] are presented. In their work, a superconducting chip with two trasmon qubits is used to simulate two-spin interaction described by the Hamiltonian

$$\hat{H}_{1,2}^{x,y} = \frac{J}{2}\left(\hat{X}_1\hat{X}_2 + \hat{Y}_1\hat{Y}_2\right) \tag{3.29}$$

This means that they where able to evolve the qubits' state during time t, using microwave pulses on the chip, with unitary dynamics governed by Hamiltonian 3.29. It is easy to see that by performing single qubit rotations, it is possible to emulate more complicated dynamics, for instance, an isotropic XYZ interaction

$$\hat{H}_{1,2}^{x,y,z} = J\left(\hat{X}_1\hat{X}_2 + \hat{Y}_1\hat{Y}_2 + \hat{Z}_1\hat{Z}_2\right) \tag{3.30}$$

This is illustrated on figure

Chapter 4

Anisotropic Spin Chain

4.1 Section 1

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Chapter 5

Variational Quantum Time Evolution

5.1 Section 1

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