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

Undergraduate Thesis

Diego Alejandro Herrera Rojas

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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.

Acknowledgements

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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. 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, simulation of a Heisenberg Hamiltonian on an arbitrary graph is considered in the context of the quantum circuit model.

Even though this Hamiltonian is far simpler than arbitrary N-qubit systems Hamiltonians, it can be readily generalized to produce interesting behavior. For instance, it is well known that a Heisenberg chain exhibits a quantum phase transition at zero temperature. In the present work, a parametric Heisenberg Model is simulated, thus opening the possibility of extending the algorithm to the field of Quantum Machine Learning.

In particular, the recently proposed Variational Quantum Thermalizer (VQT) [13] is considered for producing thermal states of a magnetic system. A Quantum Neural Network (QNN) based upon time evolution of a parametric Heisenberg Hamiltonian is used to learn the thermal states of a magnetic system in a 2D system with non-square topology. In consequence, time evolution of an elementary Hamiltonian is used to study thermal properties of a quantum system, thus illustrating the potential of digital quantum computation in material science.

After a review of the main concepts of quantum computing (chapter 2), the fundamentals of quantum time simulation are revised on chapter chapter 3. On chapter 4, the algorithm for simulating evolution of a Heisenberg spin system, with nearest neighbor interaction is presented. Simulations using Qiskit, as well as experimental results of execution on IBM Q devices are presented. Experimental and theoretical state fidelities produced by the algorithm are discussed in this chapter too. Finally, on chapter 5, a quantum neural network is implemented that computes thermal states of a spin system using the Variational Quantum Thermalizer. This QNN is based upon the algorithm devised on chapter 4.

Chapter 2

Quantum Computing

2.1 Section 1

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2.2 Section 2

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2.3 Section 3

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$$\hat{Z}\left|\psi\right\rangle = \pm\left|\psi\right\rangle \tag{2.1}$$

2.4 Section 4

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$$\exp\left(-\mathrm{i}\hat{Z}\right)\left|\psi(0)\right\rangle = \pm\left|\psi(t)\right\rangle \tag{2.2}$$

2.5 Section 5

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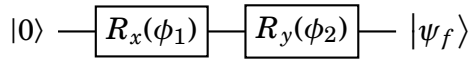

Figure 2.1: Demo circuit from quantikz

2.6 Section 6

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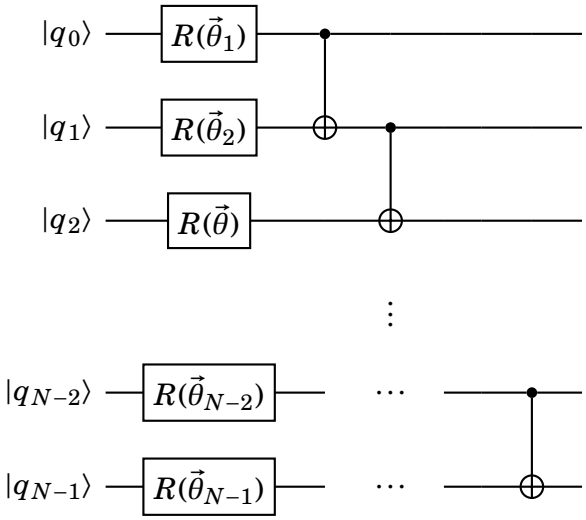

Figure 2.2: Demo larger circuit

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. [7] 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]:

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

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

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

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

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

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 discretized statevectors

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

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 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

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

Which for time-independent Hamiltonians reduces to

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

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

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

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

$$\hat{U}_P = \mathrm{e}^{-\mathrm{i}t\frac{\hat{p}^2}{2m}}$$

Is efficiently computable, using the Quantum Fourier Transform Algorithm:

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

Therefore, if operator

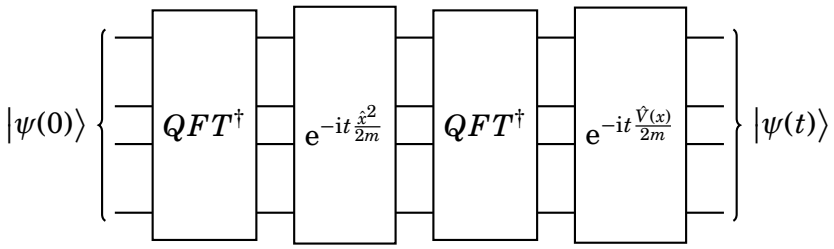

Figure 3.1: Time evolution slice for a single particle state on a digital quantum computer. This step should be repeated several times, with a time step dt, which depends upon the desired error bound and spatial discretization.

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

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

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

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, 7]. 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 [12, 6]

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

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 [12]

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

On [6], Barry et. al. show that Suzuki-Trotter shcemes can efficiently simulate sparse Hamiltonians, shuch 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

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

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 Hibert space to a 2^M-dimensional Hilbert space. In that case, the number of qubits required for siulation 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 follong section, demonstrations of this approach to the study of the Hubbard Model and the Electronic structure problem are introdeced.

3.3 Examples of Quantum Time Simulation

On section 3.1, a comparison between classical time simulation and quantum time simulation was introduced. In partiular, a scheme for integrating Schrödinger's equation for a n-particle system was proposed. The quantum evolution algorithm there introduced corresponds to standard first quantization techniques applied to the solution of many body problems [1, 10, 5]. Albeit useful in some instances, first quantization techniques are not the most effciently implemented in quantum processors.

A shortcomming of first quantization methods is that physical symmetrization properties are not taken into account. In this section, second quantization techniques for simulating many body dynamics are introduced. Systems such as magnetic solids with periodic structure, or chemical molecules have clear symmetries that can be profitted by using this formalism [8, 1, 5]. After introducing second quantization techniques in the context of such systems, their relationship to Ising-like Hamiltonians is introduced by presenting qubit mappings such as the Jordan-Wigner transform (JWT) and Bravyi-Kitaev mapping (BKM).

Chapter 4

Anisotropic Spin Chain

4.1 Section 1

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Chapter 5

Variation Quantum Thermalizer

5.1 Section 1

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