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Miriam Caron

Pitzer College

Bo Peng Dr.

Pacific Northwest National Laboratory

Scott Gould Dr.

Pitzer College

Kevin Setter Dr.

Pitzer College

Niranjan Govind Dr.

Pacific Northwest National Laboratory

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**Can the XY+Z Heisenberg Model Be Compressed Using the Yang-Baxter Equation?
An Exploration of the Compression of Quantum Time Dynamic Circuits Describing
Heisenberg Spin Chains**

A Thesis Presented

by

Miriam Caron

To the Keck Science Department
of
Claremont McKenna, Scripps, and Pitzer Colleges

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The Degree of Bachelor of Arts

Senior Thesis in Physics

12 December 2022

**Can the XY+Z Heisenberg Model Be Compressed Using the Yang-Baxter Equation? An
Exploration of the Compression of Quantum Time Dynamic Circuits Describing
Heisenberg Spin Chains**

Miriam Caron,^{1, 2, 3, a)} Bo Peng,^{3, b)} Scott Gould,^{1, 2, c)} Kevin Setter,^{1, 2, d)} and Niranjan Govind^{3, e)}

¹⁾*Pitzer College, 1050 N Mills Ave, Claremont, CA 91711*

²⁾*Keck Science Department, 925 N Mills Ave, Claremont, CA 91711*

³⁾*Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA 99352*

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Abstract

Quantum computing is currently deployed on noisy intermediate-scale quantum (NISQ) devices, which are only able to simulate circuits reliably on shallow depth quantum circuits. A promising problem on near-term quantum computers is quantum time dynamics (QTD). However, QTD circuits grow with increasing time simulations making them difficult to simulate on NISQ devices. This thesis project explores QTD simulations in variations of 1D Heisenberg spin chains with nearest-neighbor and transverse external field interactions with an eye towards studying the dynamics in broader classes of spin models. I first study the quantum Yang-Baxter equation (YBE) and how it has been shown to compress simulations of QTD of spin models without external magnetic fields and its relationship to the free fermion model. I then combine this research with similar attempts at compressing QTD simulations of spin models that include an external field like the XY+Z model. I find that the XY+Z model cannot be compressed and deployed on a NISQ device because the YBE cannot be performed on the model perfectly, however, a more generalized transverse field model can be compressed.

^{a)}Electronic mail: mcaron@students.pitzer.edu

^{b)}Electronic mail: peng398@pnnl.gov

^{c)}Electronic mail: sgould@kecksci.claremont.edu

^{d)}Electronic mail: KSetter@kecksci.claremont.edu

^{e)}Electronic mail: niri.govind@pnnl.gov

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I. INTRODUCTION

From creating more accurate weather and climate change models to streamlining drug and vaccine development¹, the ability of quantum computers to harness the properties of quantum mechanics make their development revolutionary to modern technology. Current quantum computers are considered noisy intermediate-scale quantum or NISQ devices. They operate using quantum dots, superconducting loops, ions or neutral atoms². These computers are highly susceptible to error due to their sensitivity to environmental influences and the nature of their design which means that their output are often highly noisy, hence their name.

In this thesis project I focus on the ability to preform quantum time dynamics (QTD) on NISQ devices. Since QTD result in very deep quantum circuits, it is a challenge to simulate them on quantum hardware. In other words, the shallower the quantum circuit, the less noise in the output, thus it is important to compress quantum circuits as much as possible, to make them shallow, prior to executing them on NISQ devices.² Simulating QTD on very large systems also becomes a challenge on a classical computer. Thus, this problem is well-suited for quantum computers. Quantum time dynamics give us the ability to predict the evolution of a quantum system given an initial state. In other words, QTDs describe how a Hamiltonian evolves after it has been perturbed³. The question of QTD is of high interest because it would be another step towards proving the supremacy of quantum computers over classical computers. The issue with executing QTD on a quantum computer is that their circuits are typically very deep which, as discussed earlier, leads to highly noisy outputs on NISQ devices. Because of this, it is important to compress QTD circuits as much as possible before they enter a NISQ device.

More specifically, I focus on theoretical research behind the possibility of compressing the QTD of 1D quantum Heisenberg models so that they can be deployed on NISQ devices. It is of interest to use NISQ computers to simulate the Heisenberg models as it could be a stepping ground towards more complex quantum models as well as improvements in quantum technologies⁴.

In this project I first investigate the Heisenberg Hamiltonian and it's quantum time dynamics (QTD) as well as the Yang-Baxter equation (YBE), and the free Fermion model so that I am set up with the necessary tools to understand how to compress specific variations of the Heisenberg Hamiltonian. I then closely follow Ref. 3 to understand how quantum circuits for QTD simulations of 1D-Heisenberg models can be compressed using the YBE. Specifically, 1D-Heisenberg models when no transverse field is present and the specific case when there is a transverse field but

the two interaction terms are equal. Finally, I attempt to extend this exposition to my own study of the compression to a more general Heisenberg Hamiltonian with a transverse field, specifically the XY+Z model, utilizing the YBE. Although I find that it cannot be perfectly turned over with the YBE, I am able to find an almost YBE-able model by employing a generalized Heisenberg Hamiltonian and transforming it to a free Fermion model by following the work of Ref. 5. However, because the XY+Z model is not able to be cleanly compressed it cannot be deployed on a NISQ device.

II. BACKGROUND

A. Theory

I start by reviewing the Heisenberg Hamiltonian, quantum time dynamics, the Yang-Baxter Equation, and their connections to free fermion models in order gain a full background required to understand quantum time dynamic circuit compression of 1D Heisenberg models.

1. Heisenberg Hamiltonian

The Heisenberg Hamiltonian⁶⁻⁸ is commonly used to describe the quantum mechanics of magnets organized in a lattice. The Hamiltonian can be written as

$$\hat{H} = -\sum_{\alpha} (J_{\alpha} \sum_{i=1}^{N-1} \sigma_i^{\alpha} \sigma_{i+1}^{\alpha}) - h_{\beta} \sum_i \sigma_i^{\beta}, \quad (1)$$

where α sums over $\{x, y, z\}$, J_{α} describes the exchange interaction between nearest-neighbour spins along the α -direction, σ_i^{α} is the α -Pauli operator on the i th spin, $h_{\beta}(t)$ is the time amplitude of the external magnetic field along the $\beta \in \{x, y, z\}$ direction. Although the Heisenberg Hamiltonian can describe lattices of magnets in multiple dimensions⁹, in this project we focus on 1D lattices, also known as chains, where at each lattice point is a spin as shown in figure 1. As well, the interactions are limited to nearest neighbor and external field interactions, meaning that for magnet i we only focus on it's interactions $i - 1$ and $i + 1$ as well as it's interaction with the external field h_{β} , but we do not care about it's interaction with any other spin in the chain. For the purposes of this project, we limit the spins to be $\frac{1}{2}$ spins, meaning that they can only be equal to $+1$ (oriented up) or -1 (oriented down).

The model varies by the relation between the interactions terms J_x, J_y, J_z , and the external field terms h_x, h_y , and h_z . For example, the XY variant of the model means that there exists a J_x and J_y interaction terms but not a J_z or any external field. Another variation is the $XX + Z$ model where J_x is equal to J_y and J_z is equal to zero and there does exist a external magnetic field but only in the Z direction, which is characterized by h_z .⁹

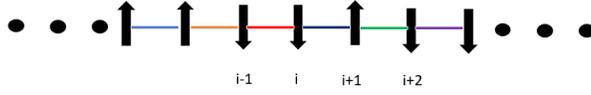


FIG. 1. A visualization of a 1D-Heisenberg spin chain, where the arrows represent the orientation of the magnets, and the colored bars represent the interactions.

2. Quantum Time Dynamics

Quantum state evolution over time^{10,11} is governed by the time-dependent Schrödinger or Dirac equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle. \quad (2)$$

The formal solution to this equation can be expressed as

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle, \quad (3)$$

where $e^{-i\hat{H}t/\hbar}$ is the evolution operator. In the 1D Heisenberg model, with the exception of $N = 2$, all the elements in the Hamiltonian do not commute with each other, thus one cannot decompose the time evolution operator as a product of two-body evolution operators.¹² In order to mitigate this, the Trotter decomposition¹³ can be used to rewrite the time evolution operator in terms of two-body components. For $N = 3$ excluding the external field, the time evolution of the Schrödinger equation is:

$$e^{-i\hat{H}t/\hbar} = \left[\left(\prod_{\alpha} e^{i\theta_{\alpha}(\sigma_1^{\alpha} \otimes \sigma_2^{\alpha} \otimes \mathbb{1})/n} \right) \times \left(\prod_{\alpha} e^{i\theta_{\alpha}(\mathbb{1} \otimes \sigma_2^{\alpha} \otimes \sigma_3^{\alpha})/n} \right) \right]^n + \mathcal{O}(t/n) \quad (4)$$

Where the Pauli matrices are defined as:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (5)$$

In order to exponentiate the Pauli matrices you can use the generalized Euler formula¹⁴

$$e^{i\cdot\theta\cdot A} = \cos(\theta) \cdot I + i \cdot \sin(\theta) \cdot A \quad (6)$$

for a matrix A. Thus you can calculate each term of the Hamiltonian as:

$$\begin{aligned}
e^{iJ_x t(\sigma_1^y \otimes \sigma_2^x)/\hbar} &= \begin{pmatrix} \cos(\theta_x) & 0 & 0 & i \sin(\theta_x) \\ 0 & \cos(\theta_x) & i \sin(\theta_x) & 0 \\ 0 & i \sin(\theta_x) & \cos(\theta_x) & 0 \\ i \sin(\theta_x) & 0 & 0 & \cos(\theta_x) \end{pmatrix} \\
e^{iJ_y t(\sigma_1^x \otimes \sigma_2^y)/\hbar} &= \begin{pmatrix} \cos(\theta_y) & 0 & 0 & -i \sin(\theta_y) \\ 0 & \cos(\theta_y) & i \sin(\theta_y) & 0 \\ 0 & i \sin(\theta_y) & \cos(\theta_y) & 0 \\ -i \sin(\theta_y) & 0 & 0 & \cos(\theta_y) \end{pmatrix} \\
e^{iJ_z t(\sigma_1^z \otimes \sigma_2^z)/\hbar} &= \begin{pmatrix} e^{i\theta_z} & 0 & 0 & 0 \\ 0 & e^{-i\theta_z} & 0 & 0 \\ 0 & 0 & e^{-i\theta_z} & 0 \\ 0 & 0 & 0 & e^{i\theta_z} \end{pmatrix}
\end{aligned} \tag{7}$$

Here, $\theta_\alpha = tJ_\alpha/\hbar$. However, the Trotter decomposition leaves us with the error term $\mathcal{O}(t/n)$ which scales linearly with time. This can be mitigated by taking a smaller step size and iterating the QTD circuit many times. This results in an overall increase in circuit depth which results in lots of noise on NISQ devices. To reduce this noise and retrieve a comprehensible output from the NISQ device the circuits must be compressed as much as possible³. In general there is only one external field present so you do not have to worry about decomposing the external field term of the Hamiltonian.

3. Yang–Baxter Equation

The Yang–Baxter equation (YBE), otherwise known as the star–triangle duality, was introduced independently in theoretical physics by Yang¹⁵ in the late 1960s and by Baxter¹⁶ in statistical mechanics in the early 1970s. In statistical mechanics, the YBE has been shown to reduce a system of four interactions, described as the star, to a system of three interactions, the triangle, without changing the total energy of the system.

Interestingly, the YBE can also be expressed in term of the third Reidemister move in knot and braid theory^{17,18}. Because the matrix corresponding to the CNOT gate can be expressed as a

braid¹⁹, the YBE can be applied to CNOT gates. Any unitary matrix \mathcal{R} can be expressed using combinations of the CNOT matrix. It follows that any quantum gate expressed as \mathcal{R} , which are required to be unitary, can be described by combinations of CNOT gates. Thus the YBE can be applied to quantum gates which I call \mathcal{R} .²⁰ The quantum YBE on three qubits is written as: Briefly, the relation is a consistency or exchange condition that allows one to factorize the interactions of three bodies into a sequence of pairwise interactions under certain conditions. Formally, this can be written as:

$$(\mathcal{R} \otimes \mathbb{1})(\mathbb{1} \otimes \mathcal{R})(\mathcal{R} \otimes \mathbb{1}) = (\mathbb{1} \otimes \mathcal{R})(\mathcal{R} \otimes \mathbb{1})(\mathbb{1} \otimes \mathcal{R}), \quad (8)$$

where the \mathcal{R} unitary gate is a operator that linearly maps $\mathcal{R} : V \otimes V \rightarrow V \otimes V$ defined as a twofold tensor product generalizing the permutation of vector space V , or a parameterized unitary gate. The quantum YBE is also referred to as turnover of gates and is necessary in order to compress quantum circuits, to make them shallower, so that they can be deployed on NISQ devices.

4. Free Fermion Model

Spins in a Heisenberg spin chain can only be up or down at every site. This property is similar to the fermion gas, where the Pauli exclusion principle requires that no two fermions with the same spin orientation can occupy the same energy level.²¹ This means that energy levels either have one or zero fermions in them. Pascual Jordan and Eugene Wigner first noticed that the sites in a Heisenberg spin chain can be thought of as energy levels of an atom. The spins pointing up or down can be thought of as full or empty energy levels in an atom as shown in equation 9 where c^\dagger is the creation operator and c is the annihilation operator, respectively.

$$|\uparrow\rangle \equiv c^\dagger |0\rangle, |\downarrow\rangle \equiv |0\rangle \quad (9)$$

Hence, the spin raising and lowering operators can be represented below in equation as 10.

$$\sigma^+ = c^\dagger = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \sigma^- = c = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \quad (10)$$

Further, the spin-raising and spin-lowering can then be re-written in terms of the transverse

spin operators as shown below in equation 11.

$$\begin{aligned}\sigma_X &= \frac{1}{2}(\sigma^+ + \sigma^-) = \frac{1}{2}(c^\dagger + c) \\ \sigma_Y &= \frac{1}{2i}(\sigma^+ - \sigma^-) = \frac{1}{2i}(c^\dagger - c)\end{aligned}\tag{11}$$

Finally, the z-component of the spin operator can be written as a combination of up and down arrows as in equation 12.

$$\sigma_z = \frac{1}{2} [|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|] \equiv c^\dagger c - \frac{1}{2}.\tag{12}$$

However, this analogy is not quite perfect because the spin operators are local operators, meaning that they only affect the (neighboring) local spins operators. However, free fermions operators are non-local meaning that they affect the operators at all sites. Jordan and Wigner accounted for this by including a phase factor called the string of all fermions.^{21,22} Put another way, the string terms keep track of the orientation of all of the previous spins and corrects the phase of the current spin. The string phase corrector is defined as $e^{i\pi\sum_{l\leq j}n_l}$ where n_l is either zero or one depending on the previous spins orientation.

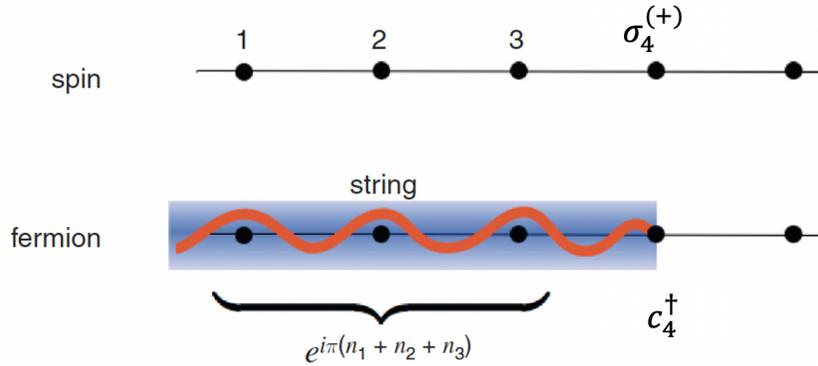


FIG. 2.²¹ An illustration of the string phase shift for the site $j = 4$ decomposed into a product of a fermion operator and a string operator.

Once the string operator is added to σ_i^+ and σ_i^- the transformation is complete to create the complete Jordan-Wigner transformations²² which are shown below in equation 13 where the operators are acting on spins i .

$$\begin{aligned}\sigma_i^+ &= c_i^\dagger e^{i\pi\sum_{l\leq j}n_l} \\ \sigma_i^- &= c_i^\dagger e^{i\pi\sum_{l\leq j}n_l} \\ \sigma_i^z &= c_i^\dagger c_i - \frac{1}{2}.\end{aligned}\tag{13}$$

The Jordan-Wigner transformation is important because it has been found that the Yang-Baxter equation can only be used on a model if and only if it can be represented as a free fermion using the Jordan-Wigner transformation.²¹ As I will discuss further, the Yang-Baxter equation will be necessary to compress a quantum circuit, therefore finding out if a model is able to be represented as a free fermion is indicative of if the resulting circuit that can be deployed on a NISQ device.

III. METHODS

A. Circuit Representation of the QTD of the Heisenberg Model Without an External Field

Due to their simplicity in form and ability to be solved exactly, I first examine the QTD circuit of 1D-Heisenberg models when no transverse field is present before adding in the transverse field later.

When no external field is present we can rewrite the Heisenberg Hamiltonian only including the components describing the interactions between the neighboring spins. I call this Hamiltonian \hat{H}_i for the interaction Hamiltonian.

$$\hat{H}_i = - \sum_{\alpha} (J_{\alpha} \sum_{i=1}^{N-1} \sigma_i^{\alpha} \sigma_{i+1}^{\alpha}), \quad (14)$$

The solution to the time dependent Schrödinger equation is given by:

$$e^{-i\hat{H}_i t/\hbar} = \prod_{\alpha} e^{iJ_{\alpha} t (\sigma_1^{\alpha} \otimes \sigma_2^{\alpha})/\hbar} + \mathcal{O}(t/n) \quad (15)$$

Combining equations (7) and (15) gives us:

$$\prod_{\alpha=x,y,z} e^{iJ_{\alpha} t (\sigma_1^{\alpha} \otimes \sigma_2^{\alpha})/\hbar} = \begin{pmatrix} e^{i\theta_z} \cos(\gamma) & 0 & 0 & ie^{i\theta_z} \sin(\gamma) \\ 0 & e^{-i\theta_z} \cos(\delta) & ie^{-i\theta_z} \sin(\delta) & 0 \\ 0 & ie^{-i\theta_z} \sin(\delta) & e^{-i\theta_z} \cos(\delta) & 0 \\ ie^{i\theta_z} \sin(\gamma) & 0 & 0 & e^{i\theta_z} \cos(\gamma) \end{pmatrix} \quad (16)$$

where $\gamma = \theta_x - \theta_y$ and $\delta = \theta_x + \theta_y$. The optimal circuit for this matrix is:

$$\prod_{\alpha} e^{iJ_{\alpha} t (\sigma_1^{\alpha} \otimes \sigma_2^{\alpha})/\hbar} = \begin{array}{c} \text{---} \bullet \text{---} \boxed{R_x(2\theta_x)} \text{---} \boxed{H} \text{---} \bullet \text{---} \boxed{S} \text{---} \boxed{H} \text{---} \bullet \text{---} \boxed{R_x(-\pi/2)} \text{---} \\ \oplus \text{---} \boxed{R_z(-2\theta_z)} \text{---} \oplus \text{---} \boxed{R_z(-2\theta_y)} \text{---} \oplus \text{---} \boxed{R_x(\pi/2)} \text{---} \end{array} \quad (17)$$

This circuit is a constant depth circuit for each time step because the number of one- and two-qubit gates does not increase with the time step.

Two commuting families of operators exist, as shown in Fig. 3, as orange and blue two-qubit gates, respectively. As mentioned in subsection II A 2, the depth of the QTD circuit grows linearly with the time step. As shown in Ref. 3, Fig. 3 shows the quantum circuit for a given time t using n

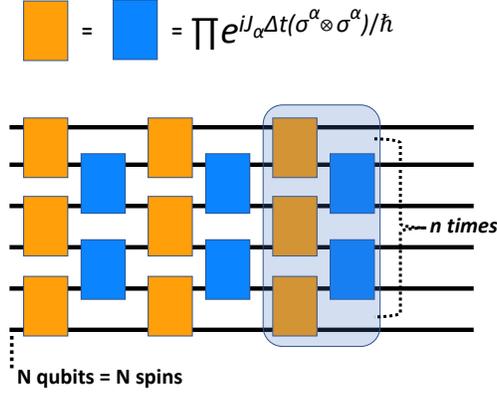


FIG. 3. Quantum circuit for time evolution of N spins, composed of n alternative layers using the Trotter approximation.³

Trotter steps. Each Trotter step is composed of a bilayer of two-qubit gates. The first layer acts on the first two qubits, followed by the third and then the fourth qubits and so on. Orange rectangles represent the first layer. The second layer of two-qubit gates starts from the second qubit and acts on the next two qubits. Blue rectangles represent the second layer. Both orange and blue rectangles combine to form an *alternative layer*, covering all possible nearest-neighbor interactions.

B. Circuit Compression of the QTD of the Heisenberg Model Without an External Field

In order to compress a QTD circuit, the circuit must satisfy the commutation, merging, and turnover (or YBE) identities²³.

1. Commutation

Commutation means that you can switch the order of gates applied to the circuit without changing the circuit. Formally defined, if two gates A and B commute then

$$A \cdot B = B \cdot A \quad (18)$$

If a quantum gate U_1 is operating on qubit i and $i + 1$ and another quantum gate U_2 is operating on $i \pm 2$ and $i \pm 2 \pm 1$, then the gates U_1 and U_2 commute because they are not acting on the same qubit. As well, if the quantum gates are representing transverse directions of the Heisenberg model then the model will commute because transverse vectors and matrices always commute.

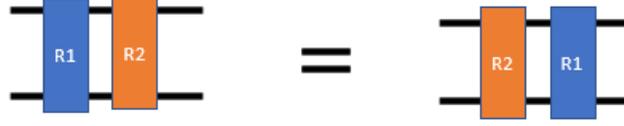


FIG. 4. Quantum circuit representation of commutation for two unitary commuting gates R1 and R2.³

2. Merge Identity

Fusion or merging means that you can combine two gates of a circuit into the same gate⁵. Merging is possible when identical gates described by different parameters act on the same qubits. For a quantum gate R the fusion identity can be written as:

$$\begin{aligned} \mathcal{R}^{ij}(\theta_x^1, \theta_y^1, \theta_z^1) \cdot \mathcal{R}^{ij}(\theta_x^2, \theta_y^2, \theta_z^2) &= \mathcal{R}^{ij}(\theta_x^3, \theta_y^3, \theta_z^3) \\ \ni \theta_x^1 + \theta_x^2 &= \theta_x^3, \theta_y^1 + \theta_y^2 = \theta_y^3, \theta_z^1 + \theta_z^2 = \theta_z^3. \end{aligned} \quad (19)$$

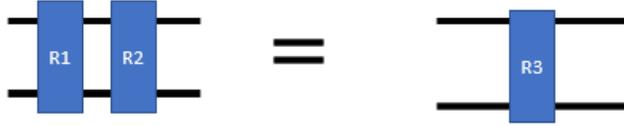


FIG. 5. Quantum circuit representation of fusion for two identical gates R1 and R2.

3. Turnover

Turnover means that for three identical quantum gates \mathcal{R} , $(1 \otimes \mathcal{R})(\mathcal{R} \otimes 1) = (1 \otimes \mathcal{R})(\mathcal{R} \otimes 1)(1 \otimes \mathcal{R})$, which was proved by the YBE discussed in subsection IIA 3.

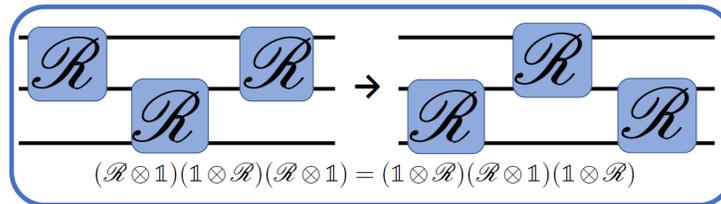


FIG. 6. Quantum circuit representation of the turnover identity.³

4. Using Reflection Symmetry and the Merge Identity to Compress a QTD Circuit

In order to compress the Heisenberg model it is first required to demonstrate reflection symmetry in a quantum circuit described by two iterations of the QTD circuit by the Trotter decomposition. Peng and co-workers³ produced figure 7 which proves reflection symmetry exists on four qubits. It should be noted that by performing these same moves, reflection symmetry can be extended to N qubits.³

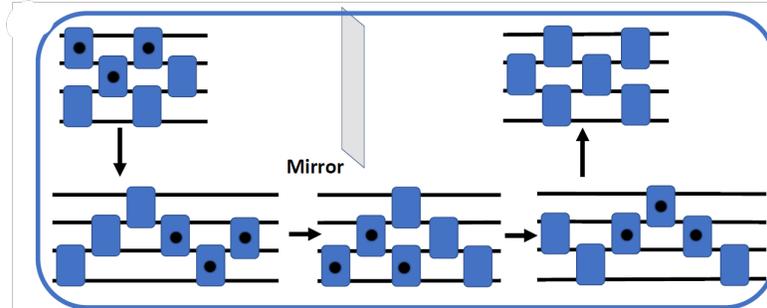


FIG. 7. Reflection symmetry is achieved by using the YBE four times on four qubits (action of YBE on which triplets is shown by black dots)³.

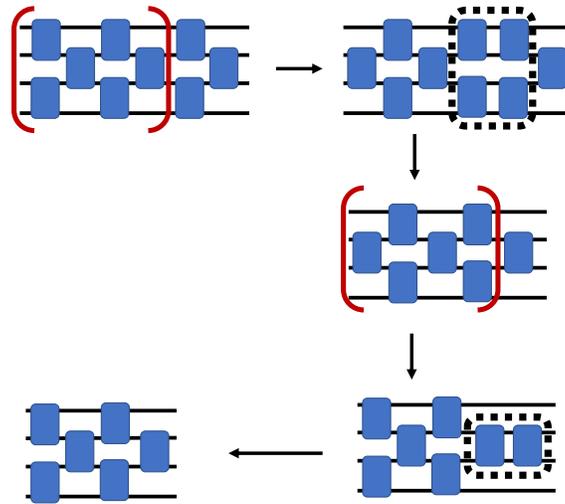


FIG. 8. Compression scheme for 4 qubits. Reflection symmetry exists with two layers of alternative gates. Addition of a third layer can be absorbed into the two layers by recursive usage of reflection symmetry (red bracket) via the YBE and merge identity (black dotted box)³.

Now that reflection symmetry has been displayed, compression of a Heisenberg model without the presence of an external field can be shown in figure 8.

The combination of reflection symmetry and the merge identity allows for the compression of N alternative layers of gates to $N/2$ alternative layers for N qubits. This is demonstrated in Ref. 3.

5. Algebraic Conditions for Reflection Symmetry

In order to determine if the reflection symmetry can be applied to a variation of the Heisenberg model the YBE needs to be satisfied. Peng and co-workers proved the following theorem for the conditions of application for the YBE on Heisenberg models without external fields.³

Theorem I: Given the time evolution operator that takes the following form, the YBE holds if and only if the following 16 relations between the γ 's and δ 's are satisfied:

$$\mathcal{R}(\gamma, \delta) = \begin{pmatrix} e^{i\delta} \cos(\gamma) & 0 & 0 & ie^{i\delta} \sin(\gamma) \\ 0 & e^{-i\delta} \cos \gamma & ie^{-i\delta} \sin \gamma & 0 \\ 0 & ie^{-i\delta} \sin \gamma & e^{-i\delta} \cos \gamma & 0 \\ ie^{i\delta} \sin(\gamma) & 0 & 0 & e^{i\delta} \cos(\gamma) \end{pmatrix}, \quad (20)$$

$$\begin{aligned}
& (\mathcal{R}(\gamma_1, \delta_1) \otimes \mathbb{1})(\mathbb{1} \otimes \mathcal{R}(\gamma_2, \delta_2))(\mathcal{R}(\gamma_3, \delta_3) \otimes \mathbb{1}) \\
& = (\mathbb{1} \otimes \mathcal{R}(\gamma_4, \delta_4))(\mathcal{R}(\gamma_5, \delta_5) \otimes \mathbb{1})(\mathbb{1} \otimes \mathcal{R}(\gamma_6, \delta_6))
\end{aligned} \tag{21}$$

$$s_{\gamma_2} c_{\gamma_1 - \gamma_3} c_{\delta_1 - \delta_3} s_{\delta_2} = c_{\gamma_5} s_{\gamma_4 + \gamma_6} s_{\delta_4 + \delta_6} c_{\delta_5} \tag{22}$$

$$c_{\gamma_2} c_{\gamma_1 - \gamma_3} c_{\delta_1 + \delta_3} s_{\delta_2} = c_{\gamma_5} c_{\gamma_4 + \gamma_6} s_{\delta_4 + \delta_6} c_{\delta_5}, \tag{23}$$

$$-s_{\gamma_2} c_{\gamma_1 + \gamma_3} s_{\delta_1 - \delta_3} c_{\delta_2} = c_{\gamma_5} s_{\gamma_4 - \gamma_6} c_{\delta_4 + \delta_6} s_{\delta_5}, \tag{24}$$

$$c_{\gamma_2} c_{\gamma_1 + \gamma_3} s_{\delta_1 + \delta_3} c_{\delta_2} = c_{\gamma_5} c_{\gamma_4 - \gamma_6} c_{\delta_4 + \delta_6} s_{\delta_5}, \tag{25}$$

$$s_{\gamma_2} c_{\gamma_1 + \gamma_3} c_{\delta_1 - \delta_3} c_{\delta_2} = c_{\gamma_5} s_{\gamma_4 + \gamma_6} c_{\delta_4 + \delta_6} c_{\delta_5}, \tag{26}$$

$$c_{\gamma_2} c_{\gamma_1 + \gamma_3} c_{\delta_1 + \delta_3} c_{\delta_2} = c_{\gamma_5} c_{\gamma_4 + \gamma_6} c_{\delta_4 + \delta_6} c_{\delta_5}, \tag{27}$$

$$-s_{\gamma_2} c_{\gamma_1 - \gamma_3} s_{\delta_1 - \delta_3} s_{\delta_2} = c_{\gamma_5} s_{\gamma_4 - \gamma_6} s_{\delta_4 + \delta_6} s_{\delta_5}, \tag{28}$$

$$c_{\gamma_2} c_{\gamma_1 - \gamma_3} s_{\delta_1 + \delta_3} s_{\delta_2} = c_{\gamma_5} c_{\gamma_4 - \gamma_6} s_{\delta_4 + \delta_6} s_{\delta_5}, \tag{29}$$

$$s_{\gamma_2} s_{\gamma_1 + \gamma_3} c_{\delta_1 - \delta_3} c_{\delta_2} = s_{\gamma_5} s_{\gamma_4 + \gamma_6} c_{\delta_4 - \delta_6} c_{\delta_5}, \tag{30}$$

$$c_{\gamma_2} s_{\gamma_1 + \gamma_3} c_{\delta_1 + \delta_3} c_{\delta_2} = s_{\gamma_5} c_{\gamma_4 + \gamma_6} c_{\delta_4 - \delta_6} c_{\delta_5}, \tag{31}$$

$$s_{\gamma_2} s_{\gamma_1 - \gamma_3} s_{\delta_1 - \delta_3} s_{\delta_2} = s_{\gamma_5} s_{\gamma_4 - \gamma_6} s_{\delta_4 - \delta_6} s_{\delta_5}, \tag{32}$$

$$-c_{\gamma_2} s_{\gamma_1 - \gamma_3} s_{\delta_1 + \delta_3} s_{\delta_2} = s_{\gamma_5} c_{\gamma_4 - \gamma_6} s_{\delta_4 - \delta_6} s_{\delta_5}, \tag{33}$$

$$-s_{\gamma_2} s_{\gamma_1 - \gamma_3} c_{\delta_1 - \delta_3} s_{\delta_2} = s_{\gamma_5} s_{\gamma_4 + \gamma_6} s_{\delta_4 - \delta_6} c_{\delta_5}, \tag{34}$$

$$-c_{\gamma_2} s_{\gamma_1 - \gamma_3} c_{\delta_1 + \delta_3} s_{\delta_2} = s_{\gamma_5} c_{\gamma_4 + \gamma_6} s_{\delta_4 - \delta_6} c_{\delta_5}, \tag{35}$$

$$-s_{\gamma_2} s_{\gamma_1 + \gamma_3} s_{\delta_1 - \delta_3} c_{\delta_2} = s_{\gamma_5} s_{\gamma_4 - \gamma_6} c_{\delta_4 - \delta_6} s_{\delta_5}, \tag{36}$$

$$c_{\gamma_2} s_{\gamma_1 + \gamma_3} s_{\delta_1 + \delta_3} c_{\delta_2} = s_{\gamma_5} c_{\gamma_4 - \gamma_6} c_{\delta_4 - \delta_6} s_{\delta_5}, \tag{37}$$

where s_p and c_p denote $\sin(p/2)$ and $\cos(p/2)$, respectively.

The proof of **Theorem I** is straightforward but lengthy and tedious if one expands both sides of Eq. (21) and performs a term-by-term comparison.³

IV. RESULTS

A. Compression of the QTD of the Heisenberg Hamiltonian With a Transverse Field

In this section I investigate the ability for 1D Heisenberg models in the presence of a transverse external field to be compressed using the same three rules (commutation, merging, and turnover) as the models without an external field. I first follow the works of refrence³ on the XX+Z model. I then try my own hand at compressing the XY+Z model.

1. XX+Z Model

The XX+Z Heisenberg model is described by the Hamiltonian

$$\hat{H} = -J_x \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x - J_x \sum_{i=1}^{N-1} \sigma_i^y \sigma_{i+1}^y - h_z \sum_{i=1}^N \sigma_i^z \quad (38)$$

Note that in this specific case $J_x = J_y$, $J_z = 0$, and $h_z \neq 0$. In the appendix of Peng et al.'s paper³ they prove that the YBE can be used on this model and thus it can be compressed to $N + 1$ layers for a N qubit system. In order to compress the model, they first break up the Hamiltonian into the external field and non-external field section of the model:

$$H = H_{XX} + H_Z \quad (39)$$

with

$$\begin{aligned} H_{XX} &= -J_x \sum_i (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y), \\ H_Z &= -h_z \sum_i \sigma_i^z. \end{aligned} \quad (40)$$

They then note that because H_{xx} and H_z are transverse, they commute. Thus $[H_{XX}, H_Z] = 0$. Because H_{xx} and H_z commute, it follows that you can decompose the QTD solution without any trotter error to

$$e^{-iHt} = e^{-iH_{XX}t} e^{-iH_Zt} = e^{-iH_Zt} e^{-iH_{XX}t} \quad (41)$$

and

$$[e^{-iH_{XX}t}, e^{-iH_Zt}] = 0. \quad (42)$$

I was able to confirm that H_{XX} and H_Z do commute by creating the matrix representations of the sub-Hamiltonians on the program Maple and check their commutability. See appendix. A to see the construction of the H_{XX} matrix representation and check it's commutation with H_Z .

Peng and coworkers demonstrate how this model is compressed in figure 9 by separating out the transverse field blocks from the interaction blocks using commutation the model forms "a circuit for pure XX model plus a single Rz layer³ ." They then invoke the same three rules for compression, commutation, merging and turnover, to compress this circuit down to $N + 1$ layers.

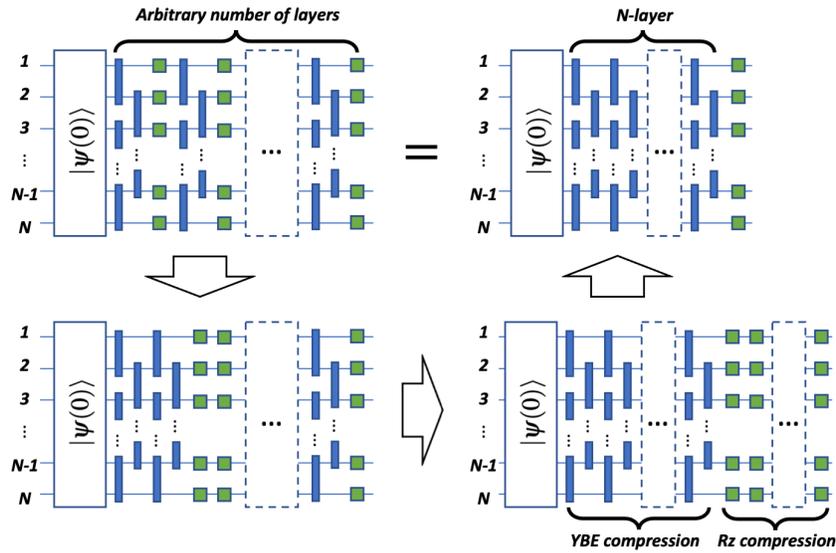


FIG. 9. Circuit compression for XX+Z model. Two-qubit gates for XX interaction are denoted by blue blocks, and single qubit Rz gates are denoted by green blocks. Note that blue and green blocks commute³.

2. XY+Z Model

The XY+Z Heisenberg model is described by the Hamiltonian

$$\hat{H} = -J_x \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x - J_y \sum_{i=1}^{N-1} \sigma_i^y \sigma_{i+1}^y - h_z \sigma_i^z \quad (43)$$

Note that in this specific case $J_x \neq J_y \neq 0, J_z = 0$ and $h_z \neq 0$.

This model differs from the XX+Z model because there are two distinct interaction terms. Figure 10 shows the circuit that describes this model on three qubits. Figure 11 shows the extension of this circuit to N qubits.

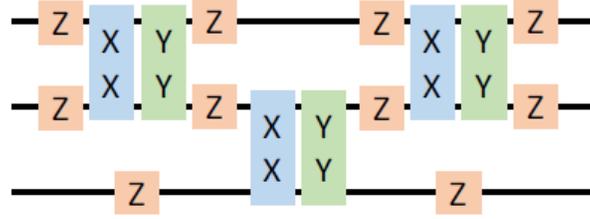


FIG. 10. The XY+Z QTD circuit for three qubits²⁴

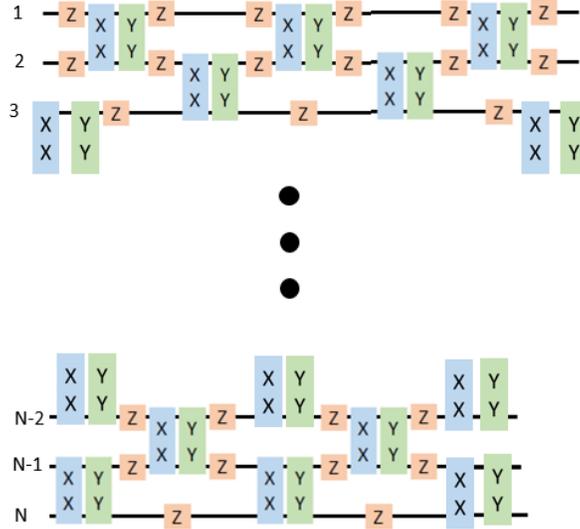


FIG. 11. The XY+Z QTD circuit for N qubits

I proposed that in order to compress this circuit you would first recognize that the interaction term in the Y direction can be re-written in terms of the X interaction and Z external field. The relationship of the $Y_i Y_{i+1}$ to $X_i X_{i+1}$ and Z_i quantum gates is shown by equation 44²³. I proved this substitution works by programming it on Maple. You can see the results of it in appendix. B.

This substitution can be represented by the circuit shown in figure 12.

$$Y_i Y_{i+1} = e^{i\frac{\pi}{4}Z_i} e^{i\frac{\pi}{4}Z_{i+1}} X_i X_{i+1} e^{-i\frac{\pi}{4}Z_i} e^{-i\frac{\pi}{4}Z_{i+1}} \quad (44)$$

Now that we see the relationship between the $Y_i Y_{i+1}$, $X_i X_{i+1}$, and Z_i gates, we can substitute $e^{i\frac{\pi}{4}Z_i} e^{i\frac{\pi}{4}Z_{i+1}} X_i X_{i+1} e^{-i\frac{\pi}{4}Z_i} e^{-i\frac{\pi}{4}Z_{i+1}}$ in for every $Y_i Y_{i+1}$ gate. This is represented by combining the circuits represented in figures 12 with 11 and replacing every green $Y_{i,i+1}$ block with a $Z_i Z_{i+1} X_i X_{i+1} Z_i Z_{i+1}$ block. This substitution is shown in the circuit represented in figure 13.

Now the circuit is entirely expressed in terms of the gates $X_i X_{i+1}$ and Z_i similar to section IV A 1

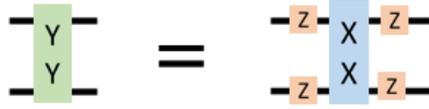


FIG. 12. The XY+Z QTD circuit for N qubits

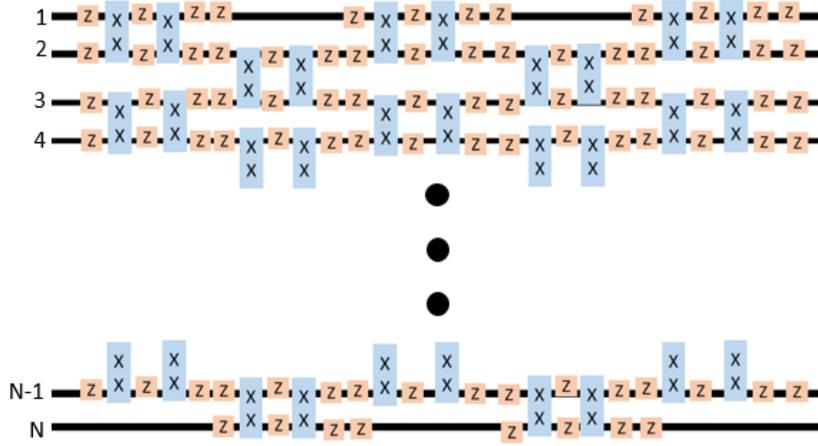


FIG. 13. The XY+Z QTD circuit for N qubits after substituting in $e^{i\frac{\pi}{4}Z_i} e^{i\frac{\pi}{4}Z_{i+1}} X_i X_{i+1} e^{-i\frac{\pi}{4}Z_i} e^{-i\frac{\pi}{4}Z_{i+1}}$ for every $Y_i Y_{i+1}$ block.

describing the $XX+Z$ model. As shown above in section IV A 1, I believed that the gates $X_i X_{i+1}$ and Z_i commute and observe the merging identity. Therefore, I proposed that once the circuit describing the $XY + Z$ is only in terms of the quantum gates $X_i X_{i+1}$ and Z_i it can be completely compressed to $N + 1$ gates. The method to compress the XY+Z QTD circuit would be similar to section IV A 1 as described in figure 9. Just like in the $XX + Z$ can, I proposed that you first separate out the $X_i X_{i+1}$ gates from the Z_i gates using commutation and then compressing the interaction gates to N gates using symmetry reflection described in and the external field gates to one singular column of gates using the merge identity.

By turning the $XY + Z$ into a $XX + Z$ like model, I analytically proposed that a complete turnover and compression is possible with the same conditions and restraints for the $XY + Z$ as for the $XX + Z$ model. It should be noted that published works²³²⁴ have analytically and numerically shown that although the $XY + Z$ model can be compressed, it is not a perfect turnover and does not quite work with the YBE.

V. DISCUSSION

A. Further Examination of the XY+Z Model

After further examination I now understand that I am not able to compress the $XY + Z$ model using the same method as the $XX+Z$ Hamiltonian sub-model. This is because when I substitute every Y block for $zzXzz$ blocks I am turning the model into a $X + Z$ model, not a $XX + Z$ model. This is demonstrated in figure 14 and proved in Appendix. B. The difference is that in the $XX + Z$ model there exists a Y block that has the same interaction term as the X block. As shown in Appendix. A, H_{XX} and H_Z commute which allows the separation and turnover required for the compression. However, H_X and H_Z without the H_Y block with the same interaction term as H_X do not commute. I figured this out by creating matrix representations in maple of H_x and H_z and checking their commutability on Maple. As you can see in Appendix. C, the matrix representations of $H_Z \cdot H_X$ is not equal to the matrix representation of $H_X \cdot H_Z$, ergo they do not commute. This means that we cannot separate out H_x and H_z required to do the compression. Therefore we cannot compress the same method as the $XX + Z$ model or preform the YBE on the $XY + Z$ model. Therefore, we cannot apply the Yang Baxter Equation to the $XY + Z$ model and it is not Yang-Baxterizable.

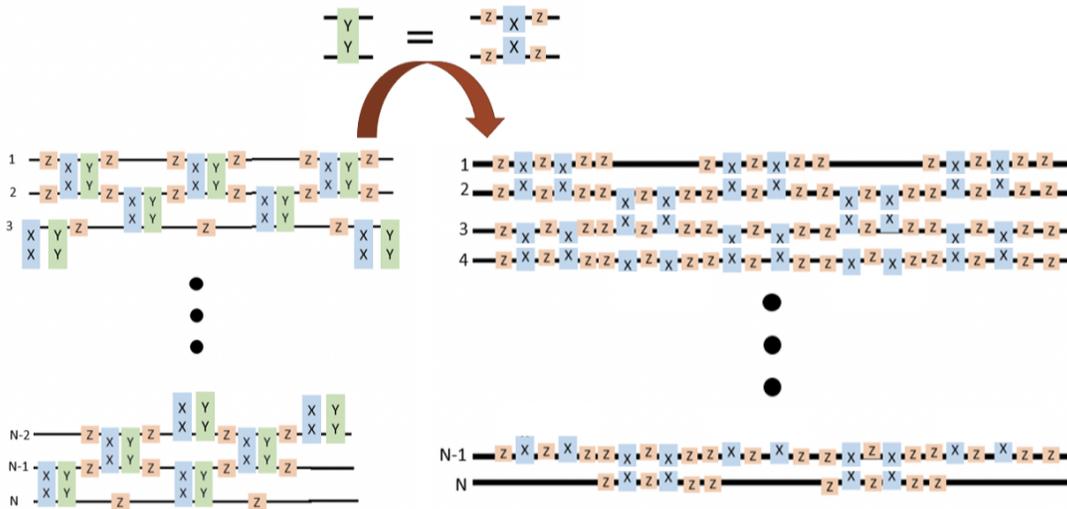


FIG. 14. The correct substitution for the XY+Z model.

B. Expressing a Yang-Baxterizable Heisenberg Model as a Free Fermion Model

As mentioned in section II A 4, if the Yang-Baxter equation can be performed on a model, that is if it is Yang-Baxterizable, then it will also be able to be transformed into a free-fermion model. I will demonstrate this for the XX+Z model that I displayed can be compressed using the Yang-Baxter equation in section IV A 1. In order to do this I will use the Jordan-Wigner transformations described in equation 13 changing the Hamiltonian from being described with spin operators to creation and annihilation operators. Using the Jordan-Wigner transformation the H_{XX} component of the XX+Z Hamiltonian described in equation 43 becomes equation 45.

$$\begin{aligned}
 H_{XX} &= -J_x \sum_i \left(\left(\frac{1}{2}(c_i^+ + c_i) \right) \left(\frac{1}{2}(c_{i+1}^+ + c_{i+1}) \right) \right. \\
 &\quad \left. + \left(\frac{1}{2i}(c_i^+ - c_i) \right) \left(\frac{1}{2i}(c_{i+1}^+ - c_{i+1}) \right) \right) \\
 &= -\frac{J_x}{2} \sum_i (c_i^+ c_{i+1} + c_{i+1} c_i^+)
 \end{aligned} \tag{45}$$

Notice that there is no string operator in the above equation 45. That is because all of the strings cancel except the $e^{i\pi n_j}$ which has no effect.

The external field in the Z-direction (H_Z) component of this Hamiltonian becomes equation 46.

$$H_z = -h_z \sum_i c_i^+ c_i + \frac{1}{2} \tag{46}$$

Combining these back together, the entire XX+Z Heisenberg Hamiltonian expressed as a free-fermion model in equation 47.

$$H_{XX+Z} = -\frac{J_x}{2} \sum_i (c_i^+ c_{i+1} + c_{i+1} c_i^+) - h_z \sum_i c_i^+ c_i + \frac{1}{2} \tag{47}$$

I have demonstrated that a Yang-Baxterizable Heisenberg model can also be converted to a free fermion model and vice versa. This is true not just for the XX+Z model, but for any Yang-Baxterizable model.²¹ This is significant because there are cases in which it is difficult to tell if a model is Yang-Baxterizable, however it is less difficult to convert it to a free fermion model. The ability to convert a Heisenberg spin model to a free fermion model is indicative of if it can be compressed and thus used on a NISQ device.

C. The Free Fermion Model of the Generalized Heisenberg Model and Its Yang Baxterability

Because non Yang-Baxterizable models cannot be transformed into free fermion models, I know that the XY+Z cannot be transformed into a free fermion model. However, we can get around this by re-writing the XY+Z model as a version of a more general Heisenberg model.²¹ The general Heisenberg model is given by equation 48.

$$H_{general} = \sum_i (a_i \sigma_i^x \sigma_{i+1}^x + b_i \sigma_i^y \sigma_{i+1}^y + f_i \sigma_i^x \sigma_{i+1}^y + d_i \sigma_i^y \sigma_{i+1}^x) + h_z \sum_i \sigma_i^z \quad (48)$$

Notice that the difference between the XY+Z model and the more general model is that here there are terms which combine σ^x and σ^y whereas in the XY+Z model there are not. To turn the $H_{general}$ model back into the XY+Z model, I would set f_i and d_i , the interaction terms of those spins, to equal zero. $H_{general}$, however can be transformed into a free fermion model. I begin this by using the Jordan-Wigner transformation as shown in equation 13 to re-express $H_{general}$ in terms of annihilation and creation operators as seen below in equation 49.

$$H_{general} = \sum_i \left[\left(\frac{a_i}{2} (c_i^\dagger + c_i) \right) \left(\frac{a_i}{2} (c_{i+1}^\dagger + c_{i+1}) \right) + \left(\frac{b_i}{2i} (c_i^\dagger - c_i) \right) \left(\frac{b_i}{2i} (c_{i+1}^\dagger - c_{i+1}) \right) + \left(\frac{f_i}{2} (c_i^\dagger + c_i) \right) \left(\frac{f_i}{2i} (c_{i+1}^\dagger - c_{i+1}) \right) + \left(\frac{d_i}{2i} (c_i^\dagger - c_i) \right) \left(\frac{d_i}{2} (c_{i+1}^\dagger + c_{i+1}) \right) \right] + h_z \sum_i c_i^\dagger c_i - \frac{1}{2}. \quad (49)$$

After expanding out the terms, $H_{general}$ can be re written as equation 50 where $\alpha = \frac{1}{4}(-if_i - id_i + a_i - b_i)$ and $\beta = \frac{1}{4}(if_i - id_i + a_i + b_i)$.

$$H_{general} = \sum_i (\alpha_i c_{i+1}^\dagger c_i^\dagger + \alpha_i^* c_{i+1} c_i + \beta_i c_{i+1} c_i^\dagger + \beta_i^* c_{i+1}^\dagger c_i) + h_z \sum_i c_i^\dagger c_i - \frac{1}{2}. \quad (50)$$

Because I have written the general Heisenberg model as a free fermion model, I know it is possible to use the Yang-Baxter equation on it. Thus if we set $f_i, d_i = 0$ and adjust α and β we could then

write the XY+Z model in terms of a free fermion model. However, by setting $f_i, d_i = 0$ it changes the structure of the free-fermion model which makes the ability for the model to turn over (implement the Yang-Baxter equation) imperfect. This imperfection makes the Yang-Baxterized XY+Z no longer a SU(2) Lie algebra like the other models which can turn over without the intermediate step of the generalized Heisenberg model.⁵ It is important that the XY+Z model is no longer a SU(2) model because it means it will not turn over perfectly, thus, it will not compress cleanly.

VI. CONCLUSIONS AND OUTLOOK

I have studied how the turn over relation, commutation and merging identity can be utilized to compress QTD circuits of 1D Heisenberg spin chains with with adjacent-neighbor and transverse field interactions from deep to shallow circuits so that they can be deployed on the current NISQ computers. I have found that along with QTD circuits describing Heisenberg models without transverse fields, the $XX+Z$ model³ can also be scaled depending on the number of spins independently of time and step size. This produces a shallow quantum circuit for efficient time dynamics simulations of 1D lattice spin chains with nearest-neighbor interactions on real quantum computers. The depth of quantum circuits for each time step is independent of time and step size and depends only on the number of spins³. Through my exposition of the subject, I found that the QTD circuits of models without a transverse field, describing N spins, can be scaled to N columns of quantum gates³ and the specific case of the $XX+Z$ model with transverse fields on N spins can be scaled down to $N + 1$ columns. I also found that any Yang-Baxterizable model can be transformed into a free fermion model. However, after looking into the topic myself, I found the $XY + Z$ model was not able to be turned over cleanly, therefore, it can not be compressed and deployed on a NISQ device or turned into a free fermion model.

There is still much to be done on this topic. I am curious about the possibility of representing commutation and the merging identity in terms of topology rules just as the turnover relation is. The purpose of this would be to then find a way to completely represent the compression of quantum circuits using braid rules which could help people with a background in topology, such as myself, find new ways to compress quantum circuits.

These applications of the techniques of commutation, merging, and turning over quantum gates in QTD circuits of the Heisenberg Hamiltonian are significant because they open up the possibility of simulating a broader class of Heisenberg models on NISQ devices in the future. As well, these results provide promising evidence for more complicated quantum models that are not able to be simulated on classical computers to do so on NISQ devices.

VII. ACKNOWLEDGMENT

I would like to thank Dr. Govind for his guidance and support throughout this project. I would also like to thank Professor Setter for his advice, Professor Gould for his assistance with Maple, and Professor Wong for sparking my interest in the subject. As well, I would like to acknowledge that I began this work while a Science Undergraduate Laboratory Intern (SULI) working at the Pacific Northwest National Laboratory and my work during that internship was funded by the Department of Energy. Lastly, I'd like to thank Muffin the big orange cat.

VIII. APPENDIX

Appendix A: Proof that H_{xx} and H_Z commute .

I used Maple to check that H_{xx} and H_Z commute. This is seen if figure 15

```

> Hxx := Hx(tx) · Hy(tx);

```

$$H_{xx} := \begin{bmatrix} \cos(\theta x)^2 + \sin(\theta x)^2 & 0 & 0 & 0 \\ 0 & \cos(\theta x)^2 - \sin(\theta x)^2 & 2i \sin(\theta x) \cos(\theta x) & 0 \\ 0 & 2i \sin(\theta x) \cos(\theta x) & \cos(\theta x)^2 - \sin(\theta x)^2 & 0 \\ 0 & 0 & 0 & \cos(\theta x)^2 + \sin(\theta x)^2 \end{bmatrix}$$

```

>
> HxxHz := Hxx · Hz :
HxxHz := simplify(HxxHz);

```

$$H_{xx}H_z := \begin{bmatrix} e^{-\frac{i}{2}\theta} H_{xx} & 0 & 0 & 0 \\ 0 & e^{-\frac{i}{2}\theta} H_{xx} & 0 & 0 \\ 0 & 0 & e^{\frac{i}{2}\theta} H_{xx} & 0 \\ 0 & 0 & 0 & e^{\frac{i}{2}\theta} H_{xx} \end{bmatrix}$$

```

> HzHxx := Hz · Hxx :
HzHxx := simplify(HzHxx);

```

$$H_zH_{xx} := \begin{bmatrix} e^{-\frac{i}{2}\theta} H_{xx} & 0 & 0 & 0 \\ 0 & e^{-\frac{i}{2}\theta} H_{xx} & 0 & 0 \\ 0 & 0 & e^{\frac{i}{2}\theta} H_{xx} & 0 \\ 0 & 0 & 0 & e^{\frac{i}{2}\theta} H_{xx} \end{bmatrix}$$

```

> Equal(HxxHz, HzHxx);

```

true

FIG. 15. The commutation of H_{xx} and H_Z

Appendix B: Proof that H_Y is equal to $H_z H_z H_X H_z H_z$

I used Maple to check that $H_Y = H_z H_z H_X H_z H_z$. This is seen if figure 16.

Appendix C: Proof that H_X and H_z do not Commute

Using Maple, I found that H_z and H_X do not commute proving that the $XY + Z$ model cannot be compressed. This is seen if figure 17.

$zz \cdot Hx \cdot zz^*$:
 $zHxz := \text{simplify}(zz \cdot Hx \cdot zz^*);$

$$zHxz := \begin{bmatrix} \cos(\theta) & 0 & 0 & -i \sin(\theta) \\ 0 & \cos(\theta) & i \sin(\theta) & 0 \\ 0 & i \sin(\theta) & \cos(\theta) & 0 \\ -i \sin(\theta) & 0 & 0 & \cos(\theta) \end{bmatrix}$$

H_y ,

$$\begin{bmatrix} \cos(\theta) & 0 & 0 & -i \sin(\theta) \\ 0 & \cos(\theta) & i \sin(\theta) & 0 \\ 0 & i \sin(\theta) & \cos(\theta) & 0 \\ -i \sin(\theta) & 0 & 0 & \cos(\theta) \end{bmatrix}$$

$\text{Equal}(zHxz, H_y);$

true

FIG. 16. $H_Y = R_z R_x H_X R_z R_x$

$xz := Hx \cdot \text{KroneckerProduct}(Rz, Rz) :$
 $xz := \text{simplify}(xz);$

$$xz := \begin{bmatrix} \cos(\theta) e^{-i\theta} & 0 & 0 & i \sin(\theta) e^{i\theta} \\ 0 & \cos(\theta) & i \sin(\theta) & 0 \\ 0 & i \sin(\theta) & \cos(\theta) & 0 \\ i \sin(\theta) e^{-i\theta} & 0 & 0 & \cos(\theta) e^{i\theta} \end{bmatrix}$$

$zx := \text{KroneckerProduct}(Rz, Rz) \cdot Hx;$
 $zx := \text{simplify}(zx);$

$$zx := \begin{bmatrix} \cos(\theta) \left(e^{-\frac{1}{2}i\theta} \right)^2 & 0 & 0 & i \sin(\theta) \left(e^{-\frac{1}{2}i\theta} \right)^2 \\ 0 & \cos(\theta) e^{-\frac{1}{2}i\theta} e^{\frac{1}{2}i\theta} & i \sin(\theta) e^{-\frac{1}{2}i\theta} e^{\frac{1}{2}i\theta} & 0 \\ 0 & i \sin(\theta) e^{-\frac{1}{2}i\theta} e^{\frac{1}{2}i\theta} & \cos(\theta) e^{-\frac{1}{2}i\theta} e^{\frac{1}{2}i\theta} & 0 \\ i \sin(\theta) \left(e^{\frac{1}{2}i\theta} \right)^2 & 0 & 0 & \cos(\theta) \left(e^{\frac{1}{2}i\theta} \right)^2 \end{bmatrix}$$

$$zx := \begin{bmatrix} \cos(\theta) e^{-i\theta} & 0 & 0 & i \sin(\theta) e^{-i\theta} \\ 0 & \cos(\theta) & i \sin(\theta) & 0 \\ 0 & i \sin(\theta) & \cos(\theta) & 0 \\ i \sin(\theta) e^{i\theta} & 0 & 0 & \cos(\theta) e^{i\theta} \end{bmatrix}$$

$\text{Equal}(xz, zx);$

false

FIG. 17. The matrix representations of $H_Z \cdot H_X$ is not equal to the matrix representation of $H_X \cdot H_Z$ thus they do not commute.

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