EXTENDING THE GRAPH FORMALISM TO HIGHER-ORDER GATES

A. Khesin  K. Ren

MIT
77 Massachusetts Ave, Cambridge, MA 02139

Received January 13, 2022
Revised October 26, 2023

We present an algorithm for efficiently simulating a quantum circuit in the graph formalism. In the graph formalism, we present states as a linear combination of graphs with Clifford operations on their vertices. We show how a $C_3$ gate such as the Toffoli gate or $\frac{\pi}{8}$ gate acting on a stabilizer state splits it into two stabilizer states. We also describe conditions for merging two stabilizer states into one. We discuss applications of our algorithm to circuit identities and finding low stabilizer rank presentations of magic states.

Keywords: pauli, clifford states, clifford hierarchy, graph state, stabilizer rank

1 Introduction

Quantum logic gates play a crucial role in quantum informatics. These gates allow a quantum circuit to behave predictably when presented with a certain quantum state by transforming this state into a desirable one. While classical computations could all be carried out using a Turing machine, the physical reality of how classical circuits are implemented makes it useful to describe classical circuits in terms of gates. Specifically, the NAND gate behaves similarly to a transistor and is considered as a sort of “fundamental” gate. The NAND gate is in fact universal, meaning all Boolean circuits can be constructed solely out of NAND gates.

It is harder to describe the concept of universality in the quantum case because quantum operations are continuous and not discrete. Notably, if we only limit ourselves to using a finite number of universal quantum gates, we will never be able to describe all possible unitary operations, as we could only ever produce a countable number of circuits. Universal quantum computation must be able to approximate unitary quantum operations with arbitrary precision.

As Aharonov showed in [1], a small set of gates, such as the Clifford and Toffoli gates, allows for universal quantum computation. It is thus desirable to not only be able to classically simulate how these gates act on quantum states, but also to do it quickly and in a small amount of space. Notably, it is worth asking how much time and space will this simulation take as a function of the number of qubits being simulated as well as of the number of operations performed.

There is a classification of operations on quantum states called the Clifford hierarchy. We call Pauli gates and Clifford gates $C_1$ and $C_2$, respectively. The Toffoli gate is in a larger set of gates called $C_3$. We wish to be able to efficiently approximate universal circuits by simulating the action of $C_3$ gates on quantum states. We can accomplish this by considering only a
particular set of quantum states called stabilizer states, which can be represented efficiently. While Clifford gates take stabilizer states to stabilizer states, $C_3$ gates take stabilizer states to linear combinations of two stabilizer states. In this paper, we show how to simulate this action efficiently both in terms of time and space, as well as how to reduce the complexity of the presentation by showing how to combine some linear combinations of two stabilizer states into one. We accomplish this by providing explicit formulas and algorithms, and we state the conditions in which the above can be applied.

The simulation of quantum circuits by using stabilizer states has been well-studied \cite{2,5}. Graph states are special types of stabilizer states that are helpful for examining the stabilizer state and its entanglement \cite{6,8}. Graph states can be useful for stabilizer simulation as they are almost as expressive as stabilizer states and are a convenient and familiar object to work with. The expression of non-stabilizer states using stabilizer states comes with a number called stabilizer rank. Minimizing stabilizer rank continues to be a subject of study for certain families of states \cite{2,5,9,10}. Some of the non-stabilizer states we will be most interested in are called magic states, and were introduced to perform non-Clifford operations on Clifford states using only special states and Clifford operations \cite{11}.

Our paper’s contribution is to merge the fields of graph states and stabilizer simulation in a way that focuses more on working with the structures of the graph in the graph states. Furthermore, our paper looks beyond stabilizer simulation to simulating states at higher levels of the Clifford hierarchy, such as magic states in $C_3$. The aim of the paper is to offer new ways of thinking regarding the perfect simulation of higher-order states by using graphs. The goal of improving runtimes of total simulations or minimizing the stabilizer rank needed for magic state simulation is left to future work. The implications of these results are that they provide new approaches to tackle questions regarding quantum computation and stabilizer rank.

In Sections II, III, and IV we introduce definitions of the Clifford hierarchy, stabilizer rank, and graph states, respectively. In Section V we state our results and show examples of how to apply them in Section VI. The proof of the main result is in Section VII and the runtime is computed in Section VIII.

\section{Clifford Hierarchy}

We first introduce a family of sets of matrices known as the Clifford hierarchy. These are key to the study of quantum circuits.

We begin by defining a fundamental set of unitary matrices, the Pauli group. Let $n$ be the number of qubits we are simulating.

**Definition A** Let $P$, the Pauli group, be the group generated by the unitary matrices $\{X, Y, Z\}$, where $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $Y = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$, and $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. We also let $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. $P$ is on the first level of the Clifford hierarchy, so we also denote it $C_1$.

The matrices $X$, $Y$, and $Z$ are called Pauli matrices, and have many nice properties.

**Remark B** The Pauli matrices obey $XY = iZ$, as well as similar expressions obtained by cyclically permuting $X$, $Y$, and $Z$. Also note that the matrices $X$, $Y$, and $Z$ are often denoted $\sigma_x$, $\sigma_y$, and $\sigma_z$, or $\sigma_1$, $\sigma_2$, and $\sigma_3$, respectively.

In general, if we wish to denote a gate $U$ applied to a specific qubit $a$ (or pair of qubits $a,b$), we will write $U_a$ (respectively, $U_{a,b}$) and it is implied that the tensor product is taken with identity matrices applied to all other qubits. Furthermore, when writing tensor products
of several matrices, we will usually omit the $\otimes$ sign for brevity.

Since unitary matrices represent quantum gates, it is useful to examine the conjugation of one matrix by another. In other words, if a circuit contains the matrix $A$, we want to know whether the matrix $B$ commutes with it, and if it doesn’t, what is the value of $C$ in the expression $BA = AC$. Equivalently, we want to know what $B$ turns into if we “pull it through” $A$. We find that $C = A^{-1}BA$.

It is now natural to examine the normalizer of $P$, the set of matrices $C$ through which we can pull a Pauli matrix and be sure to produce a Pauli matrix.

**Definition C** Let $C_2$, the Clifford group, be the normalizer of $P$, given by $C_2 = \{ U \in U(2^n) \mid U^{-1}PU = P \otimes n \}$.

As Gottesman shows in [12], $C_2$ is generated by the Hadamard gate, $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, the phase gate $S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$, and any controlled Pauli gate, such as the controlled-X gate, $CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$, which applies the $X$ gate to the target qubit if the control qubit is in the $|1\rangle$ state. When using subscripts to indicate the qubits to which the gate is applied, we write the control qubit first. The above matrix shows $CX_{1,2}$.

**Example D** The SWAP gate is a $C_2$ gate formed by $CX_{1,2} \cdot CX_{2,1} \cdot CX_{1,2}$, which swaps the values of qubits 1 and 2 and is written as $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$.

**Definition E** We define a local Clifford operation as any of the 24 matrices in $\langle H, S \rangle$, the set of matrices generated by multiplying a sequences of $H$ and $S$ matrices, which are all of the possible Clifford operations that can be applied to a single qubit.

We can further extend this idea and ask ourselves which operators map Pauli gates to the Clifford group under conjugation. This leads us to the following definition.

**Definition F** For $k \in \mathbb{N}$, let $C_k$, the operators on level $k$ of the Clifford hierarchy, be defined recursively as $C_k = \{ U \in U(2^n) \mid U^{-1}PU \subseteq C_{k-1} \}$, with the base case being $P = C_1$. Note that the Clifford group is indeed $C_2$ under this definition. Furthermore, we note that for $k > 2$, these operators do not form a group.

As discussed earlier, we can achieve universal quantum computation by just using Clifford gates and the Toffoli gate, which is in $C_3$.

**Remark G** To apply a controlled operation $U$, the matrix used is $\begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix}$. The operation $U$ is controlled by qubit 1 and applied to remaining qubits. This operation is denoted $CU$, which can be nested if $U$ is already a controlled operation. For the rest of the paper, we use the convention that if a controlled operation $CU_{a,b}$ is applied to qubits $a$ and $b$, then when $b = a$ this operation is equal to $U_a$. We will only use this for diagonal matrices $U$, for which this convention makes more intuitive sense.

The gates in $C_3$ that we study are $T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$, $CH$, $CS$, $CCX$, $CCZ$, $CSWAP$. These are the $\frac{\pi}{8}$ gate, the controlled-H gate, the controlled-S gate, the Toffoli or controlled-controlled-X gate, the controlled-controlled-Z gate, and the controlled-SWAP gate, respectively. For simplicity, we denote the set of these six $C_3$ operators as $S$.

### 3 Stabilizer Rank

When doing classical simulations, it is convenient to start the simulation with a particular state, such as $|0\rangle^\otimes n$, and then proceed by applying operations to it. In fact there is a specific
finite subset of all \( n \)-qubit states which is convenient to work with. For this we introduce the stabilizer formalism.

**Definition H** We say that a state \( |\psi\rangle \) is a stabilizer state if there exists a set of \( n \) independent operators \( U \in \mathcal{P}^{\otimes n} \) such that \( U |\psi\rangle = |\psi\rangle \). We say that the operators \( U \) stabilize \( |\psi\rangle \).

**Remark I** If \( |\psi\rangle \) is a stabilizer state and \( U \in \mathcal{C}_2 \), then \( U |\psi\rangle \) will also be a stabilizer state. Furthermore, any stabilizer state can be expressed as \( U |0\rangle^{\otimes n} \) for some \( U \in \mathcal{C}_2 \).

One of the things that make stabilizer states useful is that they can be represented efficiently. An \( n \)-qubit state requires \( 2^n \) components to represent as a state vector, but the \( n \times n \) stabilizer matrix of Pauli matrices that identify the stabilizer state only requires \( O(n^2) \) space. This exponential improvement is particularly important if the number of qubits is large.

Bearing our goal of universal quantum computation in mind, the natural question that arises now that we have defined stabilizer states is how do \( \mathcal{C}_3 \) gates act on these states.

Immediately, we see that if \( |\psi\rangle \) is a stabilizer state and \( U \in \mathcal{C}_3 \), then \( U |\psi\rangle \) will not always be a stabilizer state, as that is only true for gates in \( \mathcal{C}_2 \). In fact, presenting the action of several \( \mathcal{C}_3 \) gates on \( |\psi\rangle \) is of great interest as this lets us perform universal quantum computation, magic state distillation, and much more. For now, we need to introduce new terminology to talk about the outputs of \( \mathcal{C}_3 \) gates on stabilizer states.

**Definition J** As defined by \([2]\), let the stabilizer rank \( \chi(|\psi\rangle) \) of an \( n \)-qubit state \( |\psi\rangle \) be the smallest number \( k \) of stabilizer states \( |\phi_i\rangle \) needed to write \( |\psi\rangle = \sum_{i=1}^{k} c_i |\phi_i\rangle \). Note that \( \chi(|\psi\rangle) \geq 1 \) with equality iff \( |\psi\rangle \) is a stabilizer state. Also we observe that \( \chi(|\psi\rangle) \leq 2^n \), since the standard basis vectors are all stabilizer states.

We will later show that if \( |\psi\rangle \) is a stabilizer state and \( U \in \mathcal{S} \) is one of the \( \mathcal{C}_3 \) gates, then we can always write \( U |\psi\rangle \) as a linear combination of no more than two stabilizer states. In other words, \( \chi(U |\psi\rangle) \leq 2 \).

This is a very important point, as this means that we can present the action of a \( \mathcal{C}_3 \) gate in a circuit as a linear combination of two stabilizer states. Since matrix multiplication is linear, a second \( \mathcal{C}_3 \) gate would act on both parts independently. This means that we have reduced the problem of finding out how a series of \( \mathcal{C}_3 \) gates acts on a stabilizer state, to learning the behaviour of just one. The cost we pay for this is that our memory system must be able to store a linear combination of stabilizer states.

Presently, this means that applying \( m \) \( \mathcal{C}_3 \) gates will result in a linear combination of \( 2^m \) stabilizer states, which we would like to avoid. What we focus on is detecting when a linear combination of two stabilizer states can be merged into one. By applying such a merging operation after every application of a \( \mathcal{C}_3 \) gate, we can massively reduce the exponential growth in the space required to represent our state. However, with our current representation of stabilizer states, this merging operation would require us to identify when a linear combination of two stabilizer matrices can be merged and produce a stabilizer matrix of the sum. We are not currently aware of a method that would allow us to do this, which is why we have to turn to a different representation of stabilizer states.

### 4 Graph States

Graphs are a very versatile mathematical object and we can use them for our purposes. Specifically, we will use graphs to represent stabilizer states and then extend this representation
Extending the graph formalism to higher-order gates

Definition K A graph $G = (V, E)$ consists of a set of vertices $V$ and a set of edges $E \subseteq V \times V$ connecting those vertices. In this paper we always take $V$ to be the set of $n$ qubits numbered from 1 to $n$. By nbhd$(a)$ we denote the neighbourhood of $a$, the set of all vertices $b$ such that $(a, b) \in E$.

We can associate a specific stabilizer state with each graph.

Definition L Let the graph state of a graph $G$, $|G\rangle$, be given by the state stabilized by the operators $g_i = X_i \prod_{j \in \text{nbhd}(i)} Z_j$, $\forall i \in V$. Note that $|G\rangle$ is a stabilizer state.

However, not all stabilizer states can be expressed as graph states, which means we need to supplement our graphs with additional information. As Van de Nest et al. show in [6], any stabilizer state can be expressed as a graph state with local Clifford operations performed on the vertices (see Definition E). This means that any stabilizer state can be denoted by $U|G\rangle$ where $U \in \langle H, S \rangle$ and $G$ is a graph. Storing such a graph takes $O(1)$ additional space per qubit, as the number of local Clifford operations is fixed. Storing the entire graph takes $O(n^2)$ space.

Now what we have to do is figure out when and how we can merge a linear combination of two graphs into one.

5 Statement of results

We now present our main result. Let $S$ be $\{T, CS, CH, CCZ, CCX, CSWAP\}$, a collection of $C_3$ gates.

Theorem A Given an operator $C \in S$ and a state $U|G\rangle$, we can find two states $U_1|G_1\rangle$ and $U_2|G_2\rangle$ such that $CU|G\rangle = aU_1|G_1\rangle + bU_2|G_2\rangle$ for some $a, b \in \mathbb{C}$ in runtime $O(n^2)$.

We will prove Theorem A by means of the following algorithm, generalizing Prop. 1 of [7].

Proposition B Let $A = \text{nbhd}(1) \cup \{1\}$, and let $B$ be a set including 1. Let $k$ be an integer. Then

$$\frac{1}{\sqrt{2}} \left( I + i^k \prod_{j \in B} Z_j \right) |G\rangle = H_1Z_1 \prod_{x \in A, y \in A} CS_{x,y}^k \prod_{x \in A, y \in B} CZ_{x,y} |G\rangle. \tag{1}$$

(Note the convention from Remark G.)

Note that the expression in Proposition B may contain a $CS_{x,y}$ operator, which is a $C_3$ gate that we are not allowed to apply to a graph. We note that the product of such terms iterates over $x \in A$ and $y \in A$. Thus, for every term $x = a \neq y = b$, we will apply both $CS_{a,b}$ and $CS_{b,a}$ which multiply to $CZ_{a,b}$, the toggling of an edge. By toggling, we refer to an edge switching from being present in the graph to not present or vice versa. Meanwhile, if $x = a = y$, then by our convention $CS_{a,a} = S_a$, which is also allowed to apply. It is also of interest how some aspects of the formula, especially the $CS$ term, seem to be reminiscent of something akin to local complementation, an operation that often shows up when working with graph states [7].

We will describe the algorithm to prove Theorem A. First, Table 1 allows us to decompose gates in $S$ into the sum of two products of projectors and $C_2$ gates:

Here, a projector is a term of the form $I + P$, where $P \in \mathcal{P}^n$. Note that these are $n$-qubit projectors, so if we were to combine several of them together, it would be done by matrix multiplication and not through tensor products. In Table 1, we use tensor products to simplify
the notation of multiplying several projectors acting on different qubits. The projectors have the nice property that conjugation by a local Clifford operator gives another projector. For example,

\[ H(I + Z)H = I + X. \]  

Thus, for any local Clifford gate \( U \) and projector \( R \), we have

\[ RU |\psi\rangle = UR' |\psi\rangle, \]

where \( R' \) is another projector. With the local Clifford operations out of the way, we can now apply our merging algorithm to \( R' |\psi\rangle \). We can split \( R' = R_1 R_2 \ldots R_k \) into a matrix product of \( n \)-qubit projectors, where any products or tensor products of projectors are separated out into separate terms. We will apply \( R_k, R_{k-1}, \ldots, R_1 \) in order to \( |\psi\rangle \). Now we need to outline how to apply a single projector \( R \) to \( |\psi\rangle \).

If \( R \) is a product of \( Z \) gates, then we can directly apply the merging algorithm. Otherwise, we first apply several substitutions. First, we replace all the \( Y \)'s in \( R \) with the equivalent expression \(-iZX\). Although there are no \( Y \) operators in our set of decompositions, we show that this procedure is even more general, and is robust to changing the Pauli operators in the projectors to be arbitrary. Next, we use the identity

\[ X_a |G\rangle = \left( \prod_{b \in \text{nbhd}(a)} Z_b \right) |G\rangle \]

(4)

to remove all \( X \) gates, replacing them with \( Z \) gates on other qubits. This identity is valid because \( X_a \prod_{b \in \text{nbhd}(a)} Z_b \) is a stabilizer for the graph state \( |G\rangle \). This operation might cause \( Z \) gates to appear on other qubits that still had \( X \) gates that needed to be applied to the graph. In this case, we use the anti-commutativity of Pauli matrices to fix the order and negate the phase of the state, if necessary. Thus, we can make sure there are only \( Z \) gates left, and we can apply the merging algorithm. The application of \( R_k \) is thus another stabilizer state, and then we can apply \( R_{k-1}, R_{k-2}, \) and so on. This proves Theorem A.
6 Examples

One important concern is that our algorithm behaves well with circuit identities. For example, applying two $CCX$ gates gives the identity, but each $CCX$ would turn one stabilizer state into two, so that we end up with four stabilizer states. A robust algorithm would find a way to merge or otherwise annihilate these four stabilizer states such that only one remains. This is the content of the next two examples, which deal with the identities $CS \cdot CS = CZ$ and $CCX \cdot CCX = III$. In both cases, we should expect the output to be a single stabilizer state. The third example is related, in which we show that the stabilizer rank of the 2-qubit magic state $TT |++\rangle$ is 2 and not 4.

6.1 $CS$

Start with a stabilizer state $|\psi\rangle = U |G\rangle$. Then

$$CS|\psi\rangle = \frac{1}{2} ((I + Z)I + (I - Z)S) U |G\rangle.$$  \hfill (5)

If we apply $CS$ again then we get

$$CZ|\psi\rangle = \frac{1}{4} ((I + Z)I + (I - Z)S)^2 U |G\rangle.$$  \hfill (6)

Now, we use the identity $(I + Z)(I - Z) = 0$ and $(I \pm Z)^2 = 2(I \pm Z)$ to simplify this to

$$CZ|\psi\rangle = \frac{1}{2} ((I + Z)I + (I - Z)Z) U |G\rangle.$$  \hfill (7)

We should have four stabilizer states, but two of them (corresponding to the cross terms) collapsed to zero. We can now perform merges on $(I + Z)U |G\rangle$ and $(I - Z)U |G\rangle$ (note that $ZU$ has been changed to $U$, without loss of generality). According to the algorithm, we should first make them into

$$U \left(I \pm i^k \prod_{q \in B} Z_q\right) |G\rangle.$$  \hfill (8)

Without loss of generality, let $1 \in B$. Then the output of the algorithm will be two stabilizer states $U_1 |G'\rangle$ and $U_2 |G'\rangle$, where

$$U_1 = U_2 \prod_{a \in A} Z_a.$$  \hfill (9)

The extra $Z_a$ terms come from the powers of $CS$ in Proposition B. Thus, we can merge $U_1 |G'\rangle$ and $U_2 |G'\rangle$ into a single final state. As expected, two $CS$ gates produce a single stabilizer state.

6.2 $CCX$

Start with a stabilizer state $|\psi\rangle = U |G\rangle$. Then

$$CCX|\psi\rangle = \left(III - \frac{1}{4}(I - Z)(I - Z)(I - X)\right) U |G\rangle.$$  \hfill (10)

Apply $CCX$ again to get

$$|\psi\rangle = \left(III - \frac{1}{4}(I - Z)(I - Z)(I - X)\right)^2 U |G\rangle.$$  \hfill (11)
Let $U = (I - Z)(I - Z)(I - X)$. Then $U^2 = 8U$. Hence

$$
(I - \frac{1}{4}U)^2 = I - \frac{1}{2}U + \frac{1}{16}U^2 = I.
$$

We thus get the desired result.

To sum up, after the first CCX we get two stabilizer states. After the second, we get four states, of which three combine to zero.

### 6.3 Magic States

As discussed, being able to implement Clifford gates and $T$ gates is sufficient for universal quantum computation. In particular, certain states called magic states can be used for implementing certain non-Clifford operations using only Clifford gates [11]. One typical form for magic states is $(T | + \rangle)^\otimes n$. Consider $T_1 T_2 | + \rangle$, where $| + \rangle$ is the graph state of the empty graph on 2 vertices. As expected, one application of the algorithm leads to two stabilizer states:

$$
T_1 | + \rangle = \frac{1}{\sqrt{2}} H_1 | + \rangle + \frac{1}{\sqrt{2}} e^{i\pi/4} H_1 Z_1 | + \rangle.
$$

(13)

Applying the algorithm again, we get four stabilizer states:

$$
T_2 T_1 | + \rangle = \frac{1}{2} H_1 H_2 | + \rangle + \frac{e^{i\pi/2}}{2} H_1 H_2 Z_2 | + \rangle + \frac{e^{i\pi/2}}{2} H_1 H_2 Z_1 | + \rangle + \frac{i}{2} H_1 H_2 Z_2 | + \rangle.
$$

(14)

We can apply our merge on the first and fourth states, and the second and third states, to get

$$
T_2 T_1 | + \rangle = \frac{1}{\sqrt{2}} S_1 H_2 | G \rangle + \frac{1}{\sqrt{2}} e^{i\pi/4} H_1 Z_1 | G \rangle,
$$

(15)

where $G$ is connected on two vertices, so $| G \rangle$ is $CZ | + \rangle$. We obtain a decomposition into two stabilizer states, which agrees with the stabilizer rank of 2 found in [2]. Currently, we do not yet know of a way to match the best known bounds for larger magic states using only this merging algorithm. It is possible that for larger numbers of qubits, a more complicated sequence of transformations must be done, which might involve making the stabilizer decomposition more complicated by splitting stabilizer states apart before they can be merged together with other states in the decomposition.

### 7 Proof of Proposition B

#### 7.1 An initial simplification

We now show that if we prove Proposition B for the case of $k \in \{0, 1\}$, then the $k + 2$ case follows. Let $A' = A \setminus \{1\}$ and $B' = B \setminus \{1\}$. We assume that for $k \in \{0, 1\}$, the equation in Proposition B holds. Then, we use the following facts:

- A. $H_1$ commutes with $Z_p$ for $p \neq 1$, and $H_1 Z_1 H_1 = X_1$;
- B. Equation [1] as we assume that our merging formula holds for $k \in \{0, 1\}$;
- C. Equation [4] which allows us to convert $X_a$ to $Z_b$'s on nbhd($a$).
Extending the graph formalism to higher-order gates

\[
H_1 Z_1 \prod_{p \in A, q \in A} C S_{p, q}^{k + 2} \prod_{p \in A, q \in B} C Z_{p, q} |G\rangle
\]

\[\equiv\]

\[
X_1 \prod_{p \in A'} Z_p H_1 Z_1 \prod_{p \in A, q \in A} C S_{p, q}^{k} \prod_{p \in A, q \in B} C Z_{p, q} |G\rangle
\]

\[\equiv\]

\[
X_1 \prod_{p \in A'} Z_p \frac{1}{\sqrt{2}} \left( I + i^k \prod_{q \in B} Z_q \right) |G\rangle
\]

\[\equiv\]

\[
\prod_{p \in A'} Z_p \frac{1}{\sqrt{2}} \left( I - i^k \prod_{q \in B} Z_q \right) X_1 |G\rangle
\]

\[\equiv\]

\[
\prod_{p \in A'} Z_p \frac{1}{\sqrt{2}} \left( I - i^k \prod_{q \in B} Z_q \right) \prod_{p \in A'} Z_p |G\rangle
\]

\[\equiv\]

\[
\frac{1}{\sqrt{2}} \left( I + i^{k + 2} \prod_{q \in B} Z_q \right) |G\rangle
\]

Thus, we need to show this where \(k \in \{0, 1\}\).

7.2 Outline of Proof

To prove Proposition B, we need to verify that the input state and the output state have the same stabilizer group and global phase.

We remark that a similar result is given as Proposition 1 in [7]. However, they only prove the first of these claims. In the following, let \(\zeta\) be the \(CZ\)'s and \(\sigma\) be the \(CS\)'s in Equation 1.

7.3 Same stabilizer group

We first consider \(k = 0\). Let \(|G\rangle\) be stabilized by \(g_1, g_2, \ldots, g_n\). Let \(|\psi\rangle = \left( I + \prod_{j \in B} Z_j \right) |G\rangle\).

Then applying the Clifford operations in the RHS of Equation 1 transforms the stabilizers by conjugation into \(g'_1, g'_2, \ldots, g'_n\). Thus, we know that \(g'_1\) through \(g'_n\) stabilize the RHS of Equation 1.

We will later prove they also stabilize \(|\psi\rangle\) by first proving three claims. Define \(A' = A \setminus \{1\}\) and \(B' = B \setminus \{1\}\).

1. \(g'_1 = \prod_{j \in B} Z_j\).

2. If \(m \notin A\), then \(g'_m\) stabilizes \(|G\rangle\).

3. If \(m \in A'\), then \(g'_1 g'_m\) stabilizes \(|G\rangle\).

Before we prove the claims, we should mention a fact. The action of \(CZ_{a, b}\) on a stabilizer \(g_k\) is trivial (i.e. doesn’t affect the stabilizer) if \(k \neq a\) or \(k \neq b\), and it is multiplication by \(Z_b\) if \(k = a\), and multiplication by \(Z_a\) if \(k = b\).

To prove Claim 1, we compute the action of \(H_1 Z_1 \zeta\) on \(g_1\). This is represented in the following equation.

\[
g'_1 = (-Z_1 X_1) \cdot \prod_{p \in A'} Z_p \prod_{q \in B'} Z_q \cdot (X_1 \prod_{p \in A'} Z_p) = \prod_{q \in B} Z_q.
\]
All terms except the first and last are the action of $\zeta$:

- the $CZ_{1,q}$ and $CZ_{p,1}$ multiply $g_1$ by $Z_q$ or $Z_p$, respectively,
- the $CZ_{p,q}$ for $p, q \neq 1$ do nothing,
- the $CZ_{1,1}$ is $Z_1$, which turns $X_1$ into $-X_1$, hence the $-1$.

The first term represents the action of $H_1 Z_1$, which turns the $X_1$ into a $-Z_1$ (hence the multiplication by $-Z_1 X_1$).

**Claim 2** has two cases: $m \in B$ and $m \notin B$.

For $m \notin B$, we have $g_m' = g_m$, because neither $\zeta$ nor $H_1 Z_1$ affects $g_m$.

For $m \in B$, the action of $\zeta$ is just $\prod_{p \in A} Z_p$, since $m \notin A$. Note that the first entry in $g_m$ was $I_1$, which is now converted to $Z_1$. The action of $H_1 Z_1$ converts the $Z_1$ to $X_1$. Thus $g_m' = (X_1 Z_1) \prod_{p \in A} Z_p g_m = g_1 g_m$, which stabilizes $|G\rangle$.

**Claim 3** has two cases: $m \in B$ and $m \notin B$.

For $m \notin B$, the action of $\zeta$ gives $\prod_{q \in B} Z_q g_m$.

For $m \in B$, the action of $\zeta$ gives

$$- \prod_{p \in A} Z_p \prod_{q \in B} Z_q g_m. \tag{18}$$

Note that the first qubit is $I_1$ because the edge $(1, m)$ is toggled off. Hence, $H_1 Z_1$ acts trivially. Thus, $g_m' = \prod_{q \in B} Z_q g_m$, and so $g_1 g_m' = g_m$.

For $m \in B$, the action of $\zeta$ gives

$$g_m' = -(X_1 Z_1) \prod_{p \in A} Z_p \prod_{q \in B} Z_q g_m \tag{19}$$

and so (since $X_1$ anticommutes with $Z_1$): $g_1 g_m' = X_1 \prod_{p \in A'} Z_p g_m = g_1 g_m$. \tag{20}

This proves **Claim 3**. Now we will prove the $g_1'$ stabilize $|\psi\rangle$. First, rewrite $|\psi\rangle = (I + g_1')|G\rangle$. Thus, $g_1'$ stabilizes $|\psi\rangle$ because $g_1'(I + g_1') = I + g_1$. Also, for $m \notin A$, we have $g_m'$ stabilizes $|\psi\rangle$ because $g_m'$ commutes with $g_1'$ and

$$g_m'(I + g_1')|G\rangle = (I + g_1')g_m'|G\rangle = (I + g_1')|G\rangle. \tag{21}$$

Finally, for $m \in A$,

$$g_m'(I + g_1')|G\rangle = (I + g_1')g_1'g_m'|G\rangle = (I + g_1')|G\rangle. \tag{22}$$

This completes $k = 0$. 
7.4 The case $k = 1$

Suppose $k = 1$. We first note that

$$i \prod_{q \in B} Z_q |G\rangle = -Y_1 X_1 \prod_{q \in B'} Z_q |G\rangle = Y_1 \prod_{q \in A'} Z_q \prod_{p \in A'} Z_p |G\rangle = -Y_1 \prod_{q \in B} Z_q \prod_{p \in A} Z_p |G\rangle. \quad (23)$$

We have the following claims.

1. $g_1' = -Y_1 \prod_{q \in B} Z_q \prod_{p \in A} Z_p$.

2. If $m \notin A$, then $g_m'$ stabilizes $|G\rangle$.

3. If $m \in A'$, then $g_1'g_m'$ stabilizes $|G\rangle$.

We show $\left( I - Y_1 \prod_{q \in B} Z_q \prod_{p \in A} Z_p \right) |G\rangle$ is stabilized by $g_m'$, in a similar way to the case $k = 0$.

Before doing the computations, we observe that $S$ commutes with $Z$, so the only non-trivial action of $S$ is converting an $X$ to a $Y$. This we represent by $Y_m X_m$ when appropriate.

The proof of Claim 1 follows the same way as in the $k = 0$ case.

$$g_1' = (Y_1 X_1) \cdot \prod_{p \in A'} Z_p \cdot \prod_{q \in B'} Z_q \prod_{p \in A'} Z_p \cdot (-1) \cdot X_1 \prod_{p \in A'} Z_p = -Y_1 \prod_{q \in B'} Z_q \prod_{p \in A'} Z_p \prod_{q \in B} Z_q \prod_{p \in A} Z_p \cdot (24)$$

The second line is the action of $\zeta$ on $g_1$, and the first is the action of $\sigma$ and $H_1 Z_1$. The only $X$ that an $S$ acts on is $X_1$, which we write as $Y_1 X_1$. $H_1 Z_1$ commutes with $Y_1$ so $H_1$ acts trivially.

Claim 2 follows the same way as when $k = 0$.

Claim 3 has two cases: $m \in B$ and $m \notin B$.

For $m \notin B$, the action of $\zeta$ gives $\prod_{q \in B} Z_q g_m$, while the action of $\sigma$ gives

$$(Y_m X_m) \prod_{p \in A \setminus \{m\}} Z_p \prod_{q \in B} Z_q g_m. \quad (25)$$

Note that the operation on the first qubit is $Z_1$ because the edge $(1, m)$ is toggled twice, so it is on. Thus, $H_1 Z_1$ acts non-trivially, and

$$g_m' = (X_1 Z_1 Y_m X_m) \prod_{p \in A \setminus \{m\}} Z_p \prod_{q \in B} Z_q g_m. \quad (26)$$

As a result,

$$g_1'g_m' = -Y_1 \prod_{q \in B} Z_q \prod_{p \in A} Z_p (X_1 Z_1 Y_m X_m) \prod_{p \in A \setminus \{m\}} Z_p \prod_{q \in B} Z_q g_m = g_m. \quad (27)$$
A. Khesin and K. Ren

For $m \in B$, the action of $\zeta$ on $g_m$ gives $-\prod_{p \in A} Z_p \prod_{q \in B} Z_q g_m$, together with the action of $\sigma$ this gives

$$ (Y_m X_m) \prod_{p \in A \setminus \{m\}} Z_p \left( - \prod_{p \in A} Z_p \prod_{q \in B} Z_q \right) g_m = i \prod_{q \in B} Z_q g_m. \quad (28) $$

Note that the operation on the first qubit is $I_1$ because the edge $(1, m)$ is toggled thrice, but was on originally (since $m \in A$) and hence is now off. Thus, $H_1Z_1$ acts trivially, $g'_m = i \prod_{q \in B} Z_q g_m$, and

$$ g'_1 g'_m = -Y_1 \prod_{q \in B} Z_q \prod_{p \in A} Z_p \cdot i \prod_{q \in B} Z_q g_m = g_1 g_m. \quad (29) $$

7.5 Same global phase

We now prove that the two sides of Equation 1 have the same global phase. Let $c = \frac{1}{\sqrt{2}}$. We apply $\langle 0|$ to both sides. Also define $\langle 1| = \langle 10 \ldots 0|$. On the LHS, the $\prod Z$ acts on the $\langle 0|$ trivially, since $|0\rangle$ is a +1 eigenstate of $Z_p$ for all $p$. Furthermore, since $|G\rangle = \prod_{(a, b) \in E} CZ_{a,b}|+\rangle$ where $E$ is the edge set of $G$, and since $CZ_{a,b}$ stabilizes $|0\rangle$ and $\langle 1|$, we have

$$ \langle 0 | \prod_{(a, b) \in E} CZ_{a,b} |+\rangle = \langle 0|+\rangle = c, \quad (30) $$

$$ \langle 1 | \prod_{(a, b) \in E} CZ_{a,b} |+\rangle = \langle 1|+\rangle = c. \quad (31) $$

Thus, $\langle 0|G\rangle = \langle 1|G\rangle = c$, so

$$ \left\langle 0 \left| \frac{1}{\sqrt{2}} \left( I + i^k \prod Z \right) \right| G \right\rangle = \frac{1 + i^k}{\sqrt{2}} \cdot c. \quad (32) $$

For the RHS, we note that $|0\rangle$ is a +1 eigenstate of $Z$, $CZ$, and $CS$. We then have

$$ \left\langle 0 \left| Z_1 \prod CS_{x,y}^k \prod CZ_{x,y} \right| G \right\rangle = c. \quad (33) $$

$$ \left\langle 1 \left| Z_1 \prod CS_{x,y}^k \prod CZ_{x,y} \right| G \right\rangle = i^k \cdot c. \quad (34) $$

This is since $|10 \ldots 0\rangle$ is a $-1$, $i$, and +1 eigenstate of $Z_1$, $S_1$, everything else, respectively. Note the two $Z_1$’s in the above product; one written as $CZ_{1,1}$, which verifies Equation 31.

Thus,

$$ \left\langle 0 \left| H_1 Z_1 \prod CS_{x,y}^k \prod CZ_{x,y} \right| G \right\rangle = \frac{1 + i^k}{\sqrt{2}} \cdot c. \quad (35) $$

In summary, we proved that applying $|0\rangle$ to both sides gives the same nonzero result (since $k \neq 2$), which means the global phases are equal. This proves the correctness of our algorithm.
8 Runtime
Consider the action of a $C_3$ gate $C$ on stabilizer state $U|G\rangle$. The steps of our algorithm are:

- Express $C$ as a linear combination of two products of Pauli projectors $D + E$ and $C_2$ gates, as in Table 1.
- Form the conjugate $D' = U^{-1}DU$.
- Convert all $X$'s and $Y$'s to $Z$'s.
- Apply the merge in Proposition B.

The main contributors to the runtime are the last two steps. If $n$ is the number of qubits, we claim that our worst-case runtime is $O(n^2)$. The first two steps above take $O(n)$ time since $|\langle H, S \rangle| = 24$. Converting an $X$ or $Y$ on a qubit to $Z$'s, which must be done for each of up to two qubits (since all of the Pauli projectors we use have a small weight), requires $O(n)$ applications of $Z$, hence has $O(n)$ runtime. Lastly, applying the gates in the algorithm takes $O(|A| \cdot |A| + |A| \cdot |B|)$. Both $|A|$ and $|B|$ are $O(n)$ so we get a runtime of $O(n^2)$.

9 Conclusions
We showed how to simulate $C_3$ circuits on stabilizer states. We use a decomposition of $C_3$ operators into a sum of projectors and a merging algorithm that combines two states. We showed robustness of our algorithm with circuit identities, and we also derived a decomposition of the magic state $TT|++\rangle$ in two stabilizer states, in accordance with the known results. As further research, we can look at how our algorithm performs when computing higher-qubit magic states. We can also look to derive more cases where merging two states is possible besides the ones we found. Finally, we can look at the implications of our $C_3$ circuit simulation algorithm for universal quantum computation.

The ideas in this paper explain how to express higher-order states as a formal sum of graphs and offer a way to merge and modify these graphs. We hope that these ideas can be extended and applied to research in areas including stabilizer rank, graph states, and Clifford simulation.

Acknowledgements
The authors are grateful to Isaac Chuang for suggesting the research question and fruitful discussions as well as to Peter Shor for helpful comments and encouragement.

References