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Quantum circuit simulation is used to verify and test large quantum circuits before constructing them physically. Improving simulation saves time and resources for designing circuits. Here we study three different aspects of simulation.

Initially, we explore the method of using graph states augmented with local Clifford operations to simulate stabilizer circuit computations, which we call graph state simulation. By deriving new transformation rules on graph states, we improve upon the current widely adopted graph state simulation algorithm. At the same time, we prove that in the worst case, at least $\Omega(n^2)$ edge toggles must be performed in order to update the graph corresponding to the stabilizer state upon application of a controlled-Pauli Z gate. Our results suggest that graph state simulation is advantageous over other methods of simulation for some but not all classes of circuits.

Then, stabilizer simulation can be used to simulate arbitrary quantum circuits by representing quantum states as linear combinations of stabilizer states. To better represent stabilizer states, we discover a unique and elegant canonical form for stabilizer states based on graph states and also show how to efficiently simplify stabilizer states to canonical form.

Also, we derive a simpler formula for combining two Pauli-related stabilizer states into one and characterize all linearly dependent triplets of stabilizer states, revealing three cases, the first with two Pauli-related stabilizer states and the other two with pairwise equal inner products. We present an algorithm for computing the inner product between stabilizer states, which receives graph states augmented with Clifford operations as inputs. Our algorithm's runtime is $O(nd^2)$ where d is the maximum degree of the graph, which improves upon the previous algorithm's runtime of $O(n^3)$.

Keywords: Stabilizer formalism, graph state, Clifford operator, Pauli operator, stabilizer circuit

CONTENTS

I. INTRODUCTION

In quantum computation and quantum information, the *stabilizer formalism* is a way of working with a particular set of quantum states. The state vectors of these states are stabilized, namely belong to the eigenspace of Hermitian Pauli operators [1]. Working with these operators is much easier than working with the state vectors themselves, and their rich structure has been studied [2, 3]. The stabilizer formalism has important applications to quantum error correction and fault-tolerant quantum computation [4, 5], where it describes the codes and circuits used, and to the classical simulation of quantum circuits [6–12]. *Graph states* are a special type of stabilizer state that can be completely defined in terms of a graph. Their entanglement properties have been studied in various contexts [13]. Graph states, just like the stabilizer formalism, have many applications such as in the classical simulation of quantum circuits [14], measurement based quantum computing [15], and quantum error correction [16, 17]. Furthermore, graph states can be extended to represent all stabilizer states by applying local Clifford operators to each of the qubits [18]. In fact, only a single layer of either Hadamard or phase gates needs to be applied to a graph state to result in an arbitrary stabilizer state [19, 20]. The orbits of graph states under local Clifford operations can be generated by applying local complementation [18].

In this paper, we seek to understand stabilizer states through the lens of graph states augmented with local Clifford operations in order to improve the classical simulation of quantum circuits. Our paper consists of Section II, containing key definitions, followed by Sections III, IV, V, each containing one of our contributions.

In Section III, we find that graph states provide us with a new *canonical form* for stabilizer states, which is unique and phase sensitive. Also, the canonical form can be directly converted to a canonical circuit that prepares stabilizer states from a computational basis state. This circuit has only four blocks of Clifford gates, which is fewer than other canonical forms [3]. Our work extends upon the work done in [17, 19, 20], which shows how to simplify stabilizer graphs, graph states with at most 2 layers of Hadamard and phase operators applied to them, to *reduced form*. We show how to simplify *extended graph states*, a generalization of stabilizer graphs where each qubit can have an arbitrary local Clifford operator applied to it, to canonical form, and we also analyze runtime.

In Section IV, we present a simpler and faster algorithm for graph state simulation. Currently, the best and widely accepted algorithm is GraphSim, introduced and implemented in [14]. GraphSim applies controlled-Pauli Z gates to extended graph states by applying local complementations to graphs iteratively with many cases depending on the local Clifford operators. GraphSim is not optimized and also does not provide insight about the updated state. We develop a formula that easily and more quickly computes the updated state. In addition, using our formula, we prove the near-impossibility of improving the theoretical runtime of applying controlled-Phase Z gates. Our research confirms that graph state simulation is most useful and only better than other methods in circuits where neighboring qubits have few interactions, such as quantum error-correcting circuits [12, 14].

In Section V, we study the linear dependence of stabilizer states by fully examining the special case of the linear dependence of three stabilizer states. We extend the work of [2] by finding two new cases of linearly dependent triplets. Our characterization enables efficient algorithms for detecting linear dependence between three stabilizer states and for computing stabilizer states that are in the span of two given stabilizer states. In addition, the merging of two stabilizer states related by a Pauli operator is important for computing measurements of Pauli observables [20, 21], which we develop a simpler algorithm for.

II. THE STABILIZER AND GRAPH FORMALISMS

Here we define important notations used throughout the paper. We start by defining the operators that we use frequently in this paper. Let a *Pauli operator* P on n qubits be of the form $i^k \bigotimes_{i=1}^{n} P_i$ where $k \in \{0,1,2,3\}$ and $P_i \in \{I, X, Y, Z\}$ is a Pauli matrix. The Pauli matrices are defined as $I \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $X \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $Y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $Z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Let the set of all Pauli operators be $\mathcal{P}$, the *Pauli group*.

For some gate U, we let $CU_{a,b}$ denote the *controlled-U gate* with control qubit a and target qubit b. For example, we let $CX_{a,b}$ denote the *controlled-X* gate with control qubit a and target b, and we define $CY_{a,b}$ and $CZ_{a,b}$ similarly. We place subscripts on single-qubit operators to turn them into n-qubit operators where that operator is applied to the particular qubit referred to by the subscript, and n is contextual. For example, Z_1 would be the Pauli Z gate on qubit 1. If $a = b$, then we assume U is diagonal and let $CU_{a,a} \equiv U_a$.

Let a *Clifford operator* C on n qubits be a unitary operator on 2^n dimensional state space such that for all Pauli operators P on n qubits, $CPC^\dagger \in \mathcal{P}$. Let the set of all Clifford operators be $\mathcal{C}$, the *Clifford group*, which is generated by the *Hadamard gate* $H \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, the *phase gate* $S \equiv \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$, and any controlled-Pauli gate [4]. We call the Clifford operators C acting on a single qubit *local Clifford operators*, and these operators are generated by H and S up to global phase.

Let the n-qubit state $|\psi\rangle$ be a *stabilizer state* if there exists a set of n commuting independent Pauli operators, $\{g_1, g_2, \ldots, g_n\}$, such that for all $i \in \{1, 2, \ldots, n\}$, $g_i^2 = I$ and $g_i |\psi\rangle = |\psi\rangle$. We call the operators g_i *stabilizers*. A stabilizer state $|\psi\rangle$ is equivalently defined as a state resulting from the action of a Clifford operator C on a computational basis state [11].

For a *graph* G, we let $E(G)$ refer to the set of edges of G and $V = \{1, 2, \ldots n\} \equiv [n]$, where vertex i and qubit i are synonymous [22]. We assume our graphs are undirected and do not have loop edges or multiple edges between two qubits. Let $\mathrm{N}(i)$ be the set of neighbors of i in G not including i, where G is contextual. Let the local complementation of a graph G at qubit i, $L_i(G)$, be G except that for each pair of qubits in $\mathrm{N}(i)$, the corresponding edge is in $L_i(G)$ if and only if it is not in G.

The *graph state* of a graph G, $|G\rangle$, is the stabilizer state with stabilizers $g_i \equiv X_i \prod_{j\in \mathrm{N}(i)} Z_j$ for $1 \le i \le n$ [18]. An equivalent way of defining graph states is

$$|G\rangle \equiv \left(\prod_{(i,j)\in E(G)} CZ_{i,j}\right) |+\rangle^{\otimes n}, \tag{1}$$

where $|+\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ [18]. When $|G\rangle$ is expressed as a state vector, the global phase is fixed by assuming the amplitude of $|0\rangle^{\otimes n}$ is positive and real.

We define our terminology for stabilizer states represented as applications of local Clifford operators to graph states, which is enabled by a theorem proved in [18].

Definition II.1. An *extended graph state* is a graph state with local Clifford operators applied to it, written as $C\,|G\rangle$ where C is a tensor product of local Clifford operators.

Let the *support* of a quantum state $|\psi\rangle$ be the number of non-zero amplitudes it has when written as a state vector, and let the *support set* be the set of vectors corresponding to the computational basis states with non-zero amplitudes in $|\psi\rangle$.

These definitions enable us to examine stabilizer states from the perspective of graph states.

III. CANONICAL FORMS FOR STABILIZER STATES

A. Canonical Generator Matrix

The binary representation of the stabilizer formalism [1] associates a binary vector with each Pauli operator generator. The generators of an n-qubit stabilizer state are stored in an $n \times 2n$ generator matrix. The rows of the generator matrix are linearly independent, and a shifted inner product can be defined so that it is 0 for all pairs of distinct rows of the generator matrix. Swapping rows corresponds to swapping generators, adding a row to another corresponds to multiplying generators, and switching columns corresponds to swapping qubits. These operations can transform a generator matrix into a *canonical form*,

$$\left(\begin{array}{cc|cc} I & A & B & 0 \\ 0 & 0 & A^T & I \end{array}\right), \tag{2}$$

where B is symmetric. However, this canonical form is not unique because of the freedom in choosing how to swap qubits. Furthermore, this canonical form can be converted into the *reduced form* for extended graph states [19].

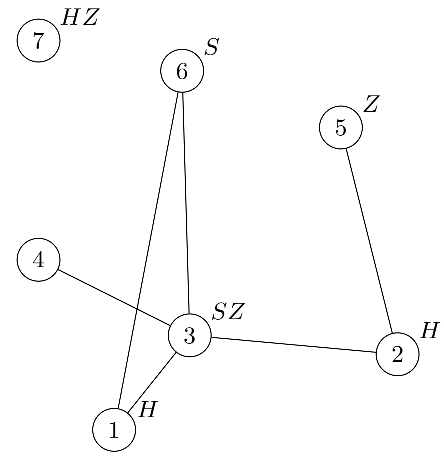


FIG. 1. An illustration of the stabilizer state in canonical form, $|\psi\rangle = H_1H_2S_3Z_3Z_5S_6H_7Z_7\,|G\rangle$, where $E(G) = \{(1,3),(1,6),(2,3),(2,5),(3,4),(3,6)\}$.

Definition III.1. Let an extended graph state $C\,|G\rangle$ be in *reduced form* if there exist n-tuples $c \equiv (c_1,\dots c_n)$ and $z \equiv (z_1,\dots z_n)$ with $c_i \in \{I,S,H\}$ and $z_i \in \{I,Z\}$ such that $C = \bigotimes_{i=1}^{n} c_i z_i$, and for all $(i,j) \in E(G)$, either $c_i \ne H$ or $c_j \ne H$.

The reduced form provides an elegant graphical representation of stabilizer states, but multiple extended graph states in reduced form can refer to the same quantum state.

B. A unique canonical form

Our canonical form is an extension of the reduced form.

Definition III.2. Let an extended graph state in reduced form be in *canonical form* if for all $(i,j) \in E(G)$ such that $c_i = H$, we have $j > i$.

The following result relates the number of H's to the support and helps us prove the canonical form is unique.

Lemma III.3. *Let* $|\psi\rangle = \bigotimes_{i=1}^{n} c_i z_i\,|G\rangle$ *be in reduced form. Let k be the number of c_i that are equal to H. Then the support of $|\psi\rangle$ is 2^{n-k}.*

Proof. Let $A \equiv \{i \in [n]\,|\,c_i = H\}$, where $k = |A|$. We use the identity $H_i CZ_{i,j} = CX_{j,i} H_i$. We also define single-qubit Pauli operators p_i as $p_i \equiv c_i z_i c_i^\dagger$. Then

$$\begin{aligned}\bigotimes_{i=1}^n c_i z_i |G\rangle &= \bigotimes_{i=1}^n p_i \prod_{i\in[n]\setminus A} (c_i)_i \prod_{i\in A} H_i |G\rangle \\ &= \bigotimes_{i=1}^n p_i \prod_{i\in[n]\setminus A} (c_i)_i \prod_{i\in A} \left(H_i \prod_{j\in \mathrm{N}(i)} CZ_{i,j} \right) \\ &\quad \cdot \prod_{(i,j)\in E(G), i\notin A, j\notin A} CZ_{i,j} |+\rangle^{\otimes n} \\ &= \bigotimes_{i=1}^n p_i \prod_{i\in[n]\setminus A} (c_i)_i \prod_{i\in A} \left(\prod_{j\in \mathrm{N}(i)} CX_{j,i} \right) \\ &\quad \cdot \prod_{(i,j)\in E(G), i\notin A, j\notin A} CZ_{i,j} \prod_{i\in A} H_i |+\rangle^{\otimes n}. \quad (3)\end{aligned}$$

$\prod_{i\in A} H_i |+\rangle^{\otimes n}$ has support 2^{n-k} because it consists of a tensor product of k $|0\rangle$'s and $n-k$ $|+\rangle$'s. The rest of Equation 3 is a product of phase operators, Pauli operators, and controlled-Pauli operators, which does not change the support of $|\psi\rangle$. □

The main advantage of our canonical form is that it uniquely represents a stabilizer state.

Theorem III.4. *If $|\psi\rangle = |\psi'\rangle$ up to global phase, and $|\psi\rangle \equiv \bigotimes_{i=1}^n c_i z_i |G\rangle$ and $|\psi'\rangle \equiv \bigotimes_{i=1}^n c_i' z_i' |G'\rangle$ are both in canonical form, then $G = G'$, $c = c'$, and $z = z'$.*

Proof. Let $A \equiv \{i \in [n] \,|\, c_i = H\}$ and $A' \equiv \{i \in [n] \,|\, c_i' = H\}$. The supports of $|\psi\rangle$ and $|\psi'\rangle$ are equal, so by Lemma III.3, $|A| = |A'| \equiv k$. Now let $A = \{a_1, a_2, \ldots a_k\}$ and $A' = \{a_1', a_2', \ldots, a_k'\}$ where $a_1 < a_2 < \cdots < a_k$, $a_1' < a_2' < \cdots < a_k'$. First, important definitions.

Definition III.5. For a binary string s and a subset $B \subset [n]$ of the same size, let $|s\rangle\langle s|_B$ be a n-qubit projector onto the subspace of n-qubit state space spanned by the basis of computational basis states that agree with s on the qubits in B. We can think of $|s\rangle\langle s|_B$ as stretching the bits in s out in a n dimensional vector to occupy the slots corresponding to qubits in B, and we let s_i denote the bit in s in the slot corresponding to qubit i.

Definition III.6. For a single-qubit state $|\varphi\rangle$ and a subset $B \subset [n]$, let $|\varphi\rangle_B$ be a tensor product of $|B|$ $|\varphi\rangle$'s, placing them in the slots corresponding to the qubits in B.

Now, suppose for the sake of contradiction $a_1 < a_1'$. We will apply projectors of the form $|s\rangle\langle s|_{[n]\setminus A}$ and $|s\rangle\langle s|_{[n]\setminus A'}$ to $|\psi\rangle$ and $|\psi'\rangle$ to derive a contradiction. Letting $Q \equiv |s\rangle\langle s|_{[n]\setminus A}$, we write

$$\begin{aligned}Q\bigotimes_{i=1}^n c_i z_i |G\rangle &= \bigotimes_{i=1}^n c_i z_i \prod_{(i,j)\in E(G)} CZ_{i,j} Q |+\rangle^{\otimes n} \quad (4)\\ &= \frac{1}{\sqrt{2^{n-k}}} \bigotimes_{i=1}^n c_i z_i \prod_{(i,j)\in E(G)} CZ_{i,j} |+\rangle_A \otimes |s\rangle \quad (5)\\ &= \frac{1}{\sqrt{2^{n-|A|}}} \bigotimes_{i=1}^n c_i z_i \prod_{(i,j)\in E(G)} Z_j^{s_i} |+\rangle_A \otimes |s\rangle \quad (6)\\ &= \frac{1}{\sqrt{2^{n-|A|}}} \bigotimes_{i=1}^n p_i \prod_{i\in[n]\setminus A} (c_i)_i |0\rangle_A \otimes |s\rangle, \quad (7)\end{aligned}$$

where Line 4 follows from the fact that Q commutes with S, Z, and CZ operators, Line 5 follows from assuming without loss of generality that $i \notin A$ due to there being no edges in G between qubits in A, and Line 7 follows by conjugating the Z operators to form Pauli operators p_i. Observe that

Proposition III.7. *For all binary strings s of length $n-k$, $|s\rangle\langle s|_{[n]\setminus A} |\psi\rangle$ and $|s\rangle\langle s|_{[n]\setminus A'} |\psi'\rangle$ are computational basis states.*

Proof. By Equation 7, $|s\rangle\langle s|_{[n]\setminus A} |\psi\rangle$ is a single computational basis state because it consists of Pauli and phase operators applied to a computational basis state, and similarly $|s\rangle\langle s|_{[n]\setminus A'} |\psi'\rangle$ is as well. □

In particular, if we consider $Q_1 \equiv |u\rangle\langle u|_{[n]\setminus A'}$, where $u_{a_1} = 1$ and the rest of the u_i equal 0, and $Q_2 \equiv |0\rangle\langle 0|_{[n]\setminus A'}$, we have

Claim III.8. *$Q_1|\psi'\rangle$ and $Q_2|\psi'\rangle$ are non-zero computational basis states that differ only in qubit a_1.*

Proof. By Line 6,

$$\begin{aligned}Q_1|\psi'\rangle &= \frac{1}{\sqrt{2^{n-k}}} \bigotimes_{i=1}^n c_i' z_i' \prod_{(i,j)\in E(G')} Z_j^{u_i} |+\rangle_{A'} \otimes |u\rangle \\ &= \frac{1}{\sqrt{2^{n-k}}} \bigotimes_{i=1}^n c_i' z_i' \prod_{j\in N_{G'}(a_1)} Z_j |+\rangle_{A'} \otimes |u\rangle \\ &= \frac{1}{\sqrt{2^{n-k}}} \prod_{j\in N_{G'}(a_1)} Z_j \bigotimes_{i=1}^n c_i' z_i' |+\rangle_{A'} \otimes |u\rangle,\end{aligned}$$

and

$$\begin{aligned}Q_2|\psi'\rangle &= \frac{1}{\sqrt{2^{n-k}}} \bigotimes_{i=1}^n c_i' z_i' \prod_{(i,j)\in E(G')} Z_j^{u_i} |+\rangle_{A'} \otimes |0\rangle_{[n]\setminus A'} \\ &= \frac{1}{\sqrt{2^{n-k}}} \bigotimes_{i=1}^n c_i' z_i' |+\rangle_{A'} \otimes |0\rangle_{[n]\setminus A'}.\end{aligned}$$

□

Let s'' be the unique binary string such that

$$|s''\rangle\langle s''|_{[n]\setminus A} Q_1 |\psi'\rangle = Q_1 |\psi'\rangle .$$

By Claim III.8, $|s''\rangle\langle s''|_{[n]\setminus A} Q_2 |\psi'\rangle = Q_2 |\psi'\rangle$. Then, the support of $|s''\rangle\langle s''|_{[n]\setminus A} |\psi'\rangle$ is at least 2. However, the support of $|s''\rangle\langle s''|_{[n]\setminus A} |\psi\rangle$ is 1 by Proposition III.7. Since $|\psi\rangle = |\psi'\rangle$, this produces the desired contradiction.

Then, we must have $a_1 = a_1'$. We cancel the H's from both sides and reduce k by 1 until k is 0. For all j, we have $c_j z_j \in \{I, S, Z, SZ\}$. If $c_j \neq c_j'$ or $z_j \neq z_j'$ for some j, then the amplitudes of $|0\rangle^{\otimes j-1} \otimes |1\rangle \otimes |0\rangle^{\otimes n-j}$ in $|\psi\rangle$ and $|\psi'\rangle$ would differ by some power of i that is not 1. Therefore, $c = c'$ and $z = z'$, and we have $|G\rangle = |G'\rangle$. If $(i,j) \in E(G)$ but $(i,j) \notin E(G')$ or vice versa, the amplitudes of $|0\rangle_{\{i,j\}} \otimes |0\rangle^{\otimes n-2}$ differ. Thus, $G = G'$. $\square$

We show that any stabilizer state can be expressed in our canonical form by a counting argument. In [11], it is proven that the number of n-qubit stabilizer states is

$$2^n \prod_{k=1}^{n} (2^k + 1). \tag{8}$$

Because our canonical form is unique, it suffices to show the following result.

Lemma III.9. *There are $2^n \prod_{k=1}^{n} (2^k+1)$ n-qubit extended graph states in canonical form.*

Proof. We wish to count all possible c, z, and G such that $c_i \in \{I, S, H\}$ and $z_i \in \{I, Z\}$ for all $i \in [n]$ and whenever $c_i = H$, all the edges in G incident to i connect to higher numbered qubits. For each qubit k, we choose c_k, z_k, and all the edges of the form (i,k) where $i < k$. If none of the $(i,k) \in E(G)$, then there are no restrictions on c_k and z_k, yielding 6 possibilities. Otherwise, the only restriction is $c_k \neq H$, and there are $2^{k-1} - 1$ possible choices for the edges, yielding $4(2^{k-1} - 1)$ possibilities. In total, there are $2^{k+1} + 2$ ways to choose c_k, z_k, and all the edges of the form (k,i) where $i < k$, and doing so for each $1 \leq k \leq n$ yields all possible extended graph state in canonical form. Thus, there are $\prod_{k=1}^{n} (2^{k+1} + 2) = 2^n \prod_{k=1}^{n} (2^k + 1)$ n-qubit extended graph states in canonical form. $\square$

C. Simplifying extended graph states

We demonstrate how to simplify extended graph states to canonical form. Like in [19], we repeatedly apply two transformation rules. The first, used in [13, 19], relates $|L_i(G)\rangle$ to $|G\rangle$.

Theorem III.10 (Van den Nest et al., Hein et al.)**.** *For any graph state $|G\rangle$ and qubit x,*

$$|G\rangle = H_x S_x^\dagger H_x \prod_{i \in \mathrm{N}(x)} S_i |L_x(G)\rangle . \tag{9}$$

The second, discovered in [19], allows us to simplify extended graph states to reduced form by eliminating pairs of H's applied to connected qubits and also allows us to simplify to canonical form by sliding H's down to smaller numbered qubits. We present our own proof in Appendix A because it uses a different methodology.

Theorem III.11 (Elliot et al.)**.** *Let $(x,y) \in E(G)$. Let $A = N(x) \cup \{x\}$ and $B = N(y) \cup \{y\}$. Then,*

$$H_x H_y |G\rangle = Z_x Z_y \prod_{p \in A, q \in B} CZ_{p,q} |G\rangle . \tag{10}$$

The runtime of the algorithm, though cubic in the worst case, can be much quicker.

Theorem III.12. *There exists an algorithm to simplify an arbitrary extended graph state, $|\psi\rangle \equiv \bigotimes_{i=1}^{n} C_i |G\rangle$, into canonical form, that runs in $O(nd^2)$, where d is the maximum degree in G encountered during the calculation.*

Proof. Multiplying both sides of Equation 9 by $S_x H_x$, we obtain

$$S_x H_x |G\rangle = H_x \prod_{p,q \in \mathrm{N}(x)} CS_{p,q} |G\rangle . \tag{11}$$

Multiplying both sides of Equation 11 by $H_x S_x H_x S_x^\dagger$, we obtain

$$\begin{aligned} H_x S_x |G\rangle &= H_x S_x H_x S_x^\dagger H_x \prod_{p,q \in \mathrm{N}(x)} CS_{p,q} |G\rangle \\ &= \frac{1+i}{\sqrt{2}} S_1^3 \prod_{p \in \mathrm{N}(x)} Z_p \prod_{p,q \in \mathrm{N}(x)} CS_{p,q} |G\rangle . \end{aligned} \tag{12}$$

Because $C_i \in \langle H, S \rangle$, each C_i is equivalent to a product of H's and S's up to global phase. Because $HH = I$ and $SS = Z$ are both Pauli operators, C_i is equivalent to a global phase and a Pauli operator applied to an alternating product of H's and S's, which we define as D_i. Thus we can write $|\psi\rangle = \alpha P \bigotimes_{i=1}^{n} D_i |G\rangle$ for some constant $\alpha \in \mathbb{C} \setminus \{0\}$ and some Pauli operator P. In what follows, we do not mention Pauli operators or global phases because we can automatically keep track of them by conjugating them through and updating α and P accordingly. We define the useful monovariant and describe an algorithm to decrease it.

Definition III.13. Let M be the sum of the total number of H's among all D_p for $1 \leq p \leq n$ and the number of p such that D_p ends in SH.

Lemma III.14. *If D_i has length at least 2, we can update D_i and all D_j for $j \in \mathrm{N}(i)$ so that M decreases.*

Proof. If D_i ends in HS, we apply Equation 12 on qubit i, which effectively removes HS from D_i and appends S onto the ends of D_i and all D_j. Otherwise, D_i ends in SH. If some D_j ends in H, we apply Theorem III.11 with $x = i, y = j$ to remove 2 H's. The last case is if all D_j end in I or S, in which case applying Equation 11 on qubit i will change D_i to not end in SH. □

Because $M \geq 0$, we can apply the updates in Lemma III.14 a finite number of times until all D_i have length at most 1, in which case $D_i \in \{I, S, H\}$ for all i. Rearranging Equation 10 and assuming $x > y$, we have

$$H_x |G\rangle = H_y Z_x Z_y \prod_{p \in A, q \in B} CZ_{p,q} |G\rangle , \qquad (13)$$

which we repeatedly apply on qubits x with D_x ending in H whenever x has a neighbor y in G with $y < x$. This must terminate since all vertices are at integers at least 1. Now $D_i \in \{I, S, H, SH\}$ for all i. For all i such that $D_i = SH$, we apply Equation 11 and simplify, not having to worry about D_j having length greater than 1 because D_j cannot end in H by assumption. After this terminates, we conjugate P through. Using the fact that $X_i |G\rangle = \prod_{p \in \mathrm{N}(i)} Z_i |G\rangle$, and $Y = -iZX$, we can turn all Y's and X's into Z's. Now, we have transformed $|\psi\rangle$ into our canonical form.

Every time we apply Theorem III.11, Equation 11, or Equation 12, we perform $O(d^2)$ edge toggles where d is the maximum degree of G. Initially, $M = O(n)$ because any local Clifford operator can be represented with a finite number of H's. Then, shortening the lengths of all the D_i to 1 takes $O(nd^2)$ operations. Next, we only need to apply Equation 13 at most $n-1$ times by applying it for $x = n, n-1, n-2, \ldots, 2$ in that order. Because the H's move to lower numbered qubits or are eliminated, the only way an H could still exist on a qubit p after the algorithm passes through p the first time is if right before the algorithm passes through p, all $q \in N(p)$ satisfy $q > p$. In that case, $N(p)$ cannot change once $x \leq p$, because p is not connected to any lower numbered qubits. Therefore, after x reaches 2, none of the H's can be moved to lower numbered qubits. Thus, moving the H's to the lowest possible numbered qubits takes $O(nd^2)$ operations. Removing all D_i that equal SH using Equation 11 takes $O(nd^2)$ operations, and simplifying the Pauli operators takes $O(nd)$ operations, so the total runtime is $O(nd^2)$. □

IV. GRAPH STATE STABILIZER SIMULATION

A. Algorithm

Graph state simulators of stabilizer circuits are advantageous in that local Clifford gates such as S and H can be applied trivially in $O(1)$ time. The bottleneck of a graph state simulator is the application of controlled-Pauli gates, such as CZ gates, which currently can be done in $O(d^2)$ time where d is the maximum degree of the graph encountered during the calculation.

To apply a gate $CZ_{x,y}$ to an extended graph state $|\psi\rangle = \bigotimes_{i=1}^{n} C_i |G\rangle$, we use the identity

$$CZ_{x,y} = \frac{1}{2} \left((I + Z_x) + (I - Z_x) Z_y \right) ,$$

conjugating the expression through the C_i so it suffices to apply operators of the form $\frac{1}{2}((I + P_x) + (I - P_x)Q_y)$ to graph states $|G\rangle$ where P_x and Q_y are Hermitian Pauli operators. This motivates the following definition.

Definition IV.1. For Hermitian Pauli operators P and Q, let $|\psi_{PQ}\rangle$ be the extended graph state obtained from simplifying the expression

$$\frac{1}{2} \left((I + P_1) + (I - P_1) Q_2 \right) |G\rangle . \qquad (14)$$

For example, $|\psi_{ZZ}\rangle$ is $CZ_{1,2} |G\rangle$, so updating G takes $O(1)$ time.

Our expressions for $|\psi_{PQ}\rangle$ and the update times based on the expressions are depicted in Table I. When $(P, Q) \in \{(Z, X), (X, X)\}$, formulas for $|\psi_{PQ}\rangle$ were computed in [19]. The rest are our own discoveries. We computed these formulas by applying Theorem V.1 and Theorem V.2. Since all the proofs are similar, they can be found in Appendix C.

B. Discussion

To apply a CZ gate to qubits x and y of the extended graph state $|\psi\rangle = \prod_{i=1}^{n} C_i |G\rangle$, GraphSim [7, 14], the currently widely adopted algorithm, performs local complementations on x, y, or neighboring qubits of x and y, changing C_x and C_y until they are both diagonal. Local complementations run in $\Omega(d^2)$, where d is the degree of the vertex at which it was applied. When applying a CZ gate using our algorithm, if $P = \pm Z$ or $Q = \pm Z$, then it takes $O(d)$ time and runs much faster than GraphSim. For example, when $C_x = HSH$ and $C_y = I$, GraphSim would perform a local complementation at qubit x, whereas our algorithm would update $|\psi\rangle$ more efficiently, based on the expression in Table I for $|\psi_{YZ}\rangle$.

(P,Q)	$\lvert\psi_{PQ}\rangle$		Update time
	$(1,2) \in E(G)$	$(1,2) \notin E(G)$	
(Z,Z)	$CZ_{1,2}\lvert G\rangle$		$O(d)$
(Z,X)	$\prod_{x \in N_2} CZ_{1,x}\lvert G\rangle$		
(Y,Z)	$S_2 Z_2 \prod_{x \in M_1} CZ_{2,x}\lvert G\rangle$		
(X,X)	$H_1 H_2 CZ_{1,2} \prod_{x \in M_1, y \in M_2} CZ_{x,y}\lvert G\rangle$	$\prod_{x \in N_1, y \in N_2} CZ_{x,y}\lvert G\rangle$	$O(d^2)$
(Y,X)	$\frac{1-i}{\sqrt{2}} \prod_{x \in M_1} S_x \; H_1 \prod_{x \in M_1 \triangle M_2} CZ_{1,x}\lvert L_1(G)\rangle$	$\prod_{x \in M_1 \triangle N_2} Z_x \prod_{x,y \in M_1 \triangle N_2} CS_{x,y} \prod_{x,y \in M_1} CS_{x,y}\lvert G\rangle$	
(Y,Y)	$-i \prod_{x,y \in M_1} CS_{x,y} \prod_{x,y \in M_2} CS_{x,y}\lvert G\rangle$	$\frac{1-i}{\sqrt{2}} \prod_{x \in M_1} S_x \; H_1 \prod_{x \in M_2} CZ_{1,x}\lvert L_1(G)\rangle$	

TABLE I. A table of formulas for $|\psi_{PQ}\rangle$, where $d = \max(\deg(1), \deg(2))$ and $\triangle$ is the symmetric difference of two sets. With this data, we can compute $|\psi_{PQ}\rangle$ for all possible unordered pairs (P,Q) since $|\psi_{PQ}\rangle$ and $|\psi_{QP}\rangle$ are equal with the roles of qubits 1 and 2 flipped, and changing the sign of P changes $|\psi_{PQ}\rangle$ by Q. Also, $N_1 \equiv \mathrm{N}(1)$, $N_2 \equiv \mathrm{N}(2)$, $M_1 \equiv N_1 \cup \{1\}$, and $M_2 \equiv N_2 \cup \{2\}$. Note that for $\{P,Q\} \in \{\{Z,Z\},\{Z,X\},\{Y,Z\}\}$, $|\psi_{PQ}\rangle$ consists of $O(d)$ CZ operators applied to $|G\rangle$, whereas for $(P,Q) \in \{\{X,X\},\{Y,X\},\{Y,Y\}\}$, $|\psi_{PQ}\rangle$ consists of $O(d^2)$ CZ operators and $O(d)$ local Clifford operators applied to $|G\rangle$, hence the $O(d^2)$ update time.

Because P and Q are each equally likely to be any of $\{\pm X, \pm Y, \pm Z\}$ during a simulation of a quantum circuit, our algorithm outperforms GraphSim approximately $\frac{5}{9}$ of the time, leading to a significant efficiency advantage when d becomes large.

In order to perform CZ updates in under quadratic time, we must find efficient update rules for $|\psi_{PQ}\rangle$ for all multi-sets $\{P,Q\} \in \{\{X,X\},\{Y,Y\},\{X,Y\}\}$. We believe such update rules cannot directly be derived by applying the graph state transformation rules, Theorems III.10 and III.11, to the expressions for $|\psi_{XX}\rangle$, $|\psi_{YX}\rangle$, and $|\psi_{YY}\rangle$ in Table I because there will always be edge toggles between two sets of vertices of size $O(d)$. In fact, we show that finding such update rules is impossible if they update the graph by toggling its edges.

Theorem IV.2. *There exists a family of extended graph states such that applying a CZ gate requires $\Omega(n^2)$ edges of G to be toggled.*

Proof. Let $A \subset [n]$ and $B \equiv [n] \setminus A$. Let $1 \in A$, $2 \in B$, $|A| = \Omega(n)$, and $|B| = \Omega(n)$. The following graphs are used in this proof.

Definition IV.3. Let $W_{i,j}$, where $i \in A$ and $j \in B$, be the graph consisting solely of edges incident to either vertex i or vertex j, such that vertex i is connected to vertex j, vertex i is connected to all vertices in $A \setminus \{i\}$, and vertex j is connected to all vertices in $B \setminus \{j\}$. Let K be the complete bipartite graph with edges between each vertex in A and each vertex in B. Let K_a (resp. K_b) be K together with all the edges between vertices in A (resp. B). Let $K_{a,i}$ (resp. $K_{b,i}$) be the graph where all the vertices in A (resp. B) are connected to each other, and vertex i is connected to every other vertex. Let G be the graph that has all possible edges, except those between vertex 2 and the vertices in A.

Suppose we want to apply $CZ_{x,y}$ to an extended graph state $|\psi\rangle \equiv \bigotimes_{i=1}^{n} C_i |G\rangle$ where $C_x = C_y = HSX$. Then, $CZ_{x,y}|\psi\rangle = \bigotimes_{i=1}^{n} C_i |\psi_{YY}\rangle$. When we update $|G\rangle$, regardless of what algorithm we use, we end up with $\bigotimes_{i=1}^{n} C_i' |G'\rangle$ for some C_i' and G' where $|G'\rangle$ is local Clifford equivalent to $|\psi_{YY}\rangle$. Applying Lemma C.5,

$$|\psi_{YY}\rangle = \frac{1-i}{\sqrt{2}} \prod_{x \in [n] \setminus \{2\}} S_x H_1 |W_{1,2}\rangle ,$$

so G' is local Clifford equivalent to $|W_{1,2}\rangle$.

Lemma IV.4. *Let R be the set of all graphs G' that are local Clifford equivalent to $|W_{1,2}\rangle$. Then*

$$R = \{K, K_a, K_b\} \cup \{K_{a,i} | i \in B\} \cup \{K_{b,i} | i \in A\} \cup \{W_{i,j} | i \in A, j \in B\}. \quad (15)$$

Proof. By a theorem proved in [18], the local Clifford equivalence of the graph states $|G'\rangle$ and $|W_{1,2}\rangle$ is equivalent to the existence of a sequence of local complementation operations taking G' to $W_{1,2}$. If we let $\mathcal{G}$ be the connected graph of graphs containing $W_{1,2}$ where edges are drawn between two graphs related by a local complementation, then $R = V(\mathcal{G})$. $\mathcal{G}$ is depicted in Figure IV B. The rest of the proof details traversing $\mathcal{G}$. For all $i \in A$ and $j \in B$,

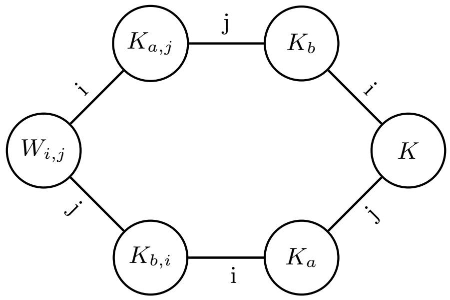


FIG. 2. A depiction of $\mathcal{G}$ in the proof of Lemma IV.4, with undirected edges labeled with the vertex that local complementation is applied to and loop edges omitted. To generate $\mathcal{G}$ in its entirely, let i and j range over all vertices in A and in B respectively.

- We consider all the edges in $\mathcal{G}$ emanating from $W_{i,j}$. For all $k \in [n] \setminus \{i, j\}$,

$$L_i(W_{i,j}) = K_{a,j}$$
$$L_j(W_{i,j}) = K_{b,i}$$
$$L_k(W_{i,j}) = W_{i,j}$$

- We consider all the edges in $\mathcal{G}$ emanating from $K_{a,j}$. The case for $K_{b,i}$ is similar. For all $k \in B \setminus \{j\}$,

$$L_i(K_{a,j}) = W_{i,j}$$
$$L_j(K_{a,j}) = K_b$$
$$L_k(K_{a,j}) = K_{a,j}$$

- We consider all the edges in $\mathcal{G}$ emanating from K, K_a, or K_b.

$$L_i(K_a) = K_{b,i}$$
$$L_j(K_a) = K$$
$$L_j(K_b) = K_{a,j}$$
$$L_i(K_b) = K$$
$$L_i(K) = K_b$$
$$L_j(K) = K_a$$

- The graph $W_{1,2}$ is connected to $W_{i,j}$ in $\mathcal{G}$.

$$L_j(L_2(L_i(L_1(W_{1,2})))) = W_{i,j}$$

□

We show that $|E(G) \triangle E(G')| = \Omega(n^2)$ for any $G' \in R$. Suppose without loss of generality that $\frac{1}{2}n \leq |A| \leq cn$ where c is some fixed constant less than 1. Then K_a has $\binom{n}{2} - \binom{|B|}{2}$ edges, which is the most number of edges out of all graphs in R.

$$\begin{aligned} |E(G) \triangle E(G')| &\geq |E(G)| - |E(G')| \\ &\geq \left(\binom{n}{2} - |A|\right) - \left(\binom{n}{2} - \binom{|B|}{2}\right) \\ &\geq \binom{|B|}{2} - |A|. \end{aligned}$$

$|E(G) \triangle E(G')| = \Omega(n^2)$ since $|B| \geq (1-c)n = \Omega(n)$. □

V. ADDITIVE PROPERTIES OF STABILIZER STATES

A. Graph merging

We first consider the case of two states related by a Pauli operator. The case when the Pauli operator acts on a single qubit was explored in [13], and the case when the Pauli operator acts on multiple qubits was explored in [20, 21]. We state the main theorem in [21] here. In [20] a related theorem is proven but without the case where k is odd.

Theorem V.1 (Khesin, Ren)**.** *Let $A = \mathrm{N}(1) \cup \{1\}$, and let B be a set including* 1*. Let k be an integer. Then*

$$\begin{aligned} &\frac{1}{\sqrt{2}} \left(I + i^k \prod_{j \in B} Z_j \right) |G\rangle \\ &\quad = H_1 Z_1 \prod_{x \in A, y \in A} CS^k_{x,y} \prod_{x \in A, y \in B} CZ_{x,y} |G\rangle . \end{aligned} \tag{16}$$

We provide an alternative formula for when k is odd that is more concise than previous formulas.

Theorem V.2. *Let $k = 2m+1$. Let A be an arbitrary set. Then*

$$\begin{aligned} (I + i^{2m+1} \prod_{p \in A} Z_p) |G\rangle &= (1 + i^{2m+1}) \\ &\cdot \prod_{p \in A} Z_p^{m+1} \prod_{p,q \in A} CS_{p,q} |G\rangle . \end{aligned} \tag{17}$$

Proof. Let $|z\rangle$ be some computational basis state, and let r be the number of i in A where the ith bit in z is 1. Let $f(r) = 1$ when $r \equiv 2 \pmod 4$ or $r \equiv 3 \pmod 4$ and 0 otherwise and $g(r) = 1$ when r is odd and 0 otherwise. Then,

$$\begin{aligned} &\langle z| (I + i^{2m+1} \prod_{p \in A} Z_p) |G\rangle \\ &\qquad = \langle z|G\rangle + i^{2m+1} (-1)^r \langle z|G\rangle, \end{aligned}$$

and

$$\begin{aligned} &\langle z| (1 + i^{2m+1}) \prod_{p \in A} Z_p^{m+1} \prod_{p,q \in A} CS_{p,q} |G\rangle \\ &\quad = (1 + i^{2m+1}) (-1)^{f(r)} (-1)^{(m+1)r} i^r |G\rangle \\ &\qquad = (1 + i^{2m+1}) i^{g(r)} (-1)^{(m+1)r} |G\rangle . \end{aligned}$$

The two expressions are equal for $m \in \{0, 1\}$ and all r. □

The merging formulas, Theorem V.1 and Theorem V.2, can be used to compute measurements of Pauli operators on extended graph states, by conjugating Pauli projectors through the local Clifford operators. These formulas can also be used to prove the correctness of the expressions for $|\psi_{PQ}\rangle$ in Table I, which we do in Appendix C.

Considering ways to merge stabilizer states that are not related by a Pauli operator, an interesting formula arises when x and y are not connected in Theorem III.11.

Theorem V.3. *Let x and y be two vertices of G that are not connected. Let $A = \mathrm{N}(x) \cup \{x\}$ and $B = \mathrm{N}(y) \cup \{y\}$. Then*

$$H_x H_y |G\rangle = Z_x Z_y |G\rangle + \prod_{p \in \mathrm{N}(x)} Z_p \prod_{q \in \mathrm{N}(y)} Z_q \prod_{x \in A, y \in B} CZ_{x,y} |G\rangle . \quad (18)$$

The proof is technical and included in Appendix A.

B. Linearly Dependent Triplets

We now turn our attention to characterizing linearly dependent triplets of stabilizer states. The following theorem shows that there are three types.

Theorem V.4. *Let $\mathcal{S} \equiv \{|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle\}$ be a set of linearly dependent stabilizer states that are not all parallel. Then, up to global phase, one of the three cases must be true*

1. *For some stabilizer state $|\phi\rangle$ and some Pauli operator P,*
$$\mathcal{S} = \{|\phi\rangle, P|\phi\rangle, \frac{I+P}{\sqrt{2}}|\phi\rangle\}. \quad (19)$$
2. *For some Clifford operator C, $1 \leq x \leq n$, and an extended graph state in reduced form $|\psi\rangle$ such that x is the only value of i such that $c_i \neq H$ and $z_i = I$ whenever $c_i = H$,*
$$\mathcal{S} = \{C|0^n\rangle, C|\psi\rangle, C(S_x|\psi\rangle)\}. \quad (20)$$
3. *For some Clifford operator C, $1 \leq x < y \leq n$, and an extended graph state in reduced form $|\psi\rangle$ such that x and y are the only two values of i such that $c_i \neq H$ and $z_i = I$ whenever $c_i = H$,*
$$\mathcal{S} = \{C|0\rangle^{\otimes n}, C|\psi\rangle, C(Z_x Z_y CZ_{x,y}|\psi\rangle)\}. \quad (21)$$

Proof. Let U be a Clifford operator such that $|\psi_1\rangle = U|0\rangle^{\otimes n}$. Let $|\psi\rangle \equiv U^\dagger|\psi_2\rangle$ and $|\varphi\rangle \equiv U^\dagger|\psi_3\rangle$. Any stabilizer state can be represented up to global phase as

$$\frac{1}{\sqrt{|V|}} \sum_{x \in V} i^{l(x)} (-1)^{q(x)} |x\rangle ,$$

where V is an affine subspace of $\mathbb{F}_2^n$, $\ell(x)$ is a linear binary function on n bits, and $q(x)$ is a quadratic binary function on n bits. Let $(V, \ell(x), q(x))$ be the corresponding triple for $|\psi\rangle$. Without loss of generality let the first non-zero amplitudes in $|\psi\rangle$ and $|\varphi\rangle$ be positive real numbers. The linear dependence of the state vectors in $\mathcal{S}$ is equivalent to the existence of $\alpha, \beta \in \mathbb{C} \setminus \{0\}$ such that

$$\frac{1}{\sqrt{|V|}} |0\rangle^{\otimes n} + \alpha |\psi\rangle = \beta |\varphi\rangle .$$

Note that $|V|$ is a power of 2. If $|V|= 1$, $|\psi\rangle$ is a non-zero computational basis state. Since the non-zero amplitudes in stabilizer states differ from each other by powers of i, α must be a power of i, $\alpha|\psi\rangle$ and $|0^n\rangle$ are Pauli related, and $|\varphi\rangle = \frac{|0^n\rangle + \alpha|\psi\rangle}{\sqrt{2}}$.

From now on assume $|V|> 1$. Then $0^n \in V$ or else $|\varphi\rangle$ would have $|V|+1 \neq 2^m$ non-zero amplitudes and could not be a stabilizer state. Also note the support set of $|\varphi\rangle$ is either V or $V \setminus \{0^n\}$, and $|V|-1 \neq 2^m \quad \forall m \geq 2$. Therefore, the only case when the support set of $|\varphi\rangle$ is $V \setminus \{0^n\}$ is if $|V|= 2$ and $\alpha = -1$, in which case $|\varphi\rangle$ is a computational basis state, related by a Pauli operator to $|0\rangle^{\otimes n}$.

From now on the support set of $|\varphi\rangle$ is V. Then, $\beta = 1 + \alpha$ and by comparing non-zero amplitudes of the left and right hand sides, $\frac{\alpha}{1+\alpha} = i^k$ for some $k \in \{1, 2, 3\}$.

Claim V.5. *If $|V|\geq 8$ and $k = 2$, it is not possible for $|\varphi\rangle$ to be a stabilizer state.*

Proof. Suppose $|\varphi\rangle$ was a stabilizer state. We consider the stabilizer state $|\phi\rangle$ with support set V and quadratic and linear functions equal to the difference of the quadratic and linear functions of $|\varphi\rangle$ and $|\psi\rangle$. The un-normalized amplitudes of $|\phi\rangle$ are equal to the ratios of the amplitudes of $|\varphi\rangle$ and $|\psi\rangle$, which are i^k for all non-zero computational basis states and 1 for $|0^n\rangle$. We use the following proposition to derive a contradiction.

Proposition V.6. *Let $|\phi\rangle$ be a stabilizer state. Then for any Pauli operator P, $\langle\phi| P |\phi\rangle \in \{0, 1, i, -1, -i\}$.*

Proof. Let $|\phi\rangle = C|0^n\rangle$ for some Clifford operator C. Then, for some Pauli operator P', $\langle\phi| P |\phi\rangle = \langle 0^n| C^\dagger P C |0^n\rangle = \langle 0^n| P' |0^n\rangle \in \{0, 1, i, -1, -i\}$. □

That $0^n \in V$ implies V is a subspace of $\mathbb{F}_2^n$. Let $e \equiv e_1 e_2 \ldots e_n$ be a basis vector of V. Let $P \equiv \bigotimes_{i=1}^n X_i^{e_i}$. Then $P|\phi\rangle = \frac{1}{\sqrt{|V|}}\left(|e\rangle - \sum_{x \in V \setminus \{e\}} |x\rangle\right)$, so $\langle\phi| P |\phi\rangle = \frac{|V|-4}{|V|} \notin \{0, 1, i, -1, -i\}$, contradicting Proposition V.6. □

Claim V.7. *If $|V|\geq 4$ and $k \in \{1, 3\}$, it is not possible for $|\varphi\rangle$ to be a stabilizer state.*

Proof. As in Claim V.5, define $|\phi\rangle$ equal to the stabilizer state whose un-normalized amplitudes are the ratios of the amplitudes of $|\varphi\rangle$ and $|\psi\rangle$, in which case $|\phi\rangle \propto |0^n\rangle \pm i \sum_{x \in V \setminus \{0^n\}} |x\rangle$. It is known that in a stabilizer state with its first non-zero amplitude positive and real, the number of pure imaginary amplitudes must be 0 or half of the support. $|\phi\rangle$ does not satisfy this condition, the desired contradiction. $\square$

By Claims V.5 and V.7, the remaining cases either satisfy $|V|= 2$ or $|V|= 4$ and $k = 2$. If $|V|= 2$, then $|\psi\rangle$ and $|\varphi\rangle$ are of the form $|\psi\rangle = \frac{|0^n\rangle + i^h |s\rangle}{\sqrt{2}}$ and $|\varphi\rangle = \frac{|0^n\rangle + i^{k+h}|s\rangle}{\sqrt{2}}$ for some h and computational basis state $|s\rangle$. Also, $|0^n\rangle = -\sqrt{2}\alpha |\psi\rangle + \sqrt{2}(1+\alpha)|\varphi\rangle$. If $k = 2$, then $\alpha = -\frac{1}{2}$ and $-2\alpha |\psi\rangle$ and $2(1+\alpha)|\varphi\rangle$ are Pauli related stabilizer states such that their sum divided by $\sqrt{2}$ is $|0^n\rangle$. If $k = 1$, then $\alpha = \frac{i-1}{2}$. If we express $|\psi\rangle$ in reduced form, then $n-1$ of the c_i are equal to H by Lemma III.3, and we can let x be the unique index i such that $c_i \neq H$. By Proposition V.10, since $\langle 0^n | \psi\rangle \neq 0$, for each $c_i = H$, we have $z_i = I$. Note that $s_x = 1$ by Lemma III.7, so $S_x |\psi\rangle = |\varphi\rangle$, and we have

$$|0^n\rangle = \frac{1-i}{\sqrt{2}} |\psi\rangle + \frac{1+i}{\sqrt{2}} S_x |\psi\rangle ,$$

which corresponds to Case 2. If $k = 3$, then similar arguments yield the same result with the roles of $|\psi\rangle$ and $|\varphi\rangle$ swapped.

If $|V|= 4$ and $k = 2$, then $\alpha = -\frac{1}{2}$ and $\beta = \frac{1}{2}$. If we express $|\psi\rangle$ in reduced form, then $n-2$ of the c_i are equal to H by Lemma III.3, and we can let x and y be the indices i such that $c_i \neq H$. By Proposition V.10, since $\langle 0^n | \psi\rangle \neq 0$, for each $c_i = H$, we have $z_i = I$. By Lemma III.7, we can write the computational basis states in $|\varphi\rangle$ and $|\psi\rangle$ as $|i\rangle_x \otimes |j\rangle_y \otimes |s_{ij}\rangle$ for $i, j \in \{0, 1\}$ and binary strings of length $n-2$ s_{ij}. We compute

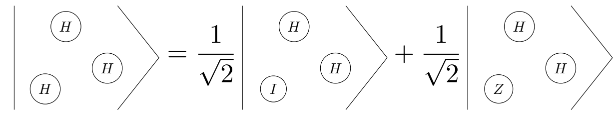
$$\begin{aligned} &\langle i|_x \otimes \langle j|_y \otimes \langle s_{ij}| Z_x Z_y C Z_{x,y} |\psi\rangle \\ &\qquad = (-1)^{1-(1-i)(1-j)} \langle i|_x \otimes \langle j|_y \otimes \langle s_{ij}| \, |\psi\rangle , \end{aligned}$$

so we have

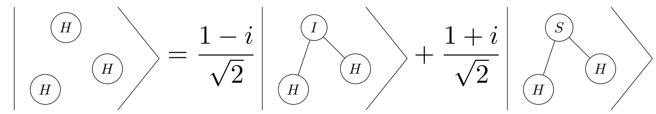
$$|0\rangle^{\otimes n} = |\psi\rangle + Z_x Z_y C Z_{x,y} |\psi\rangle ,$$

which corresponds to Case 3. $\square$

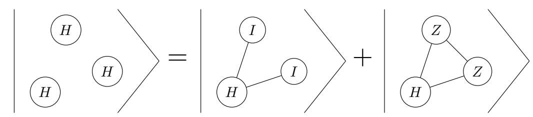
Example V.8. Small illustrative examples of each of the three cases in Theorem V.4 are shown. Each of the stabilizer states is in canonical form with vertex 1 being the lowest node in the diagram and vertex 3 being the highest.



(22)



(23)



(24)

We take a closer look at Cases 2 and 3 of Theorem V.4 by considering inner products, revealing the symmetries in non-Pauli-related triplets of linearly dependent stabilizer states.

Theorem V.9. *If two stabilizer states $|\psi_1\rangle$ and $|\psi_2\rangle$ satisfy $\langle \psi_1 | \psi_2\rangle \in \{\frac{i-1}{2}, -\frac{1}{2}\}$, then $|\psi_3\rangle$, defined as $|\psi_3\rangle \equiv -(|\psi_1\rangle + |\psi_2\rangle)$, is a stabilizer state and satisfies $\langle \psi_2 | \psi_3\rangle = \langle \psi_3 | \psi_1\rangle = \langle \psi_1 | \psi_2\rangle$.*

Proof. Let $|\psi_1\rangle = C|0^n\rangle$ and $|\psi\rangle \equiv C^\dagger |\psi_2\rangle$ for some Clifford operator C. If $\langle 0^n | \psi\rangle = \frac{i-1}{2}$, then $|\psi\rangle$ is of the form $\frac{i-1}{2}|0^n\rangle + i^k \frac{i-1}{2}|s\rangle$ for some non-zero computational basis state $|s\rangle$ and integer k. Then, $|\psi_3\rangle$, which is equal to $C(-\frac{i+1}{2}|0^n\rangle - i^k \frac{i-1}{2}|s\rangle)$, is a stabilizer state and satisfies $\langle \psi_2 | \psi_3\rangle = \langle \psi_3 | \psi_1\rangle = \frac{i-1}{2}$. Likewise, if $\langle 0^n | \psi\rangle = -\frac{1}{2}$, then $|\psi\rangle$ is of the form $-\frac{1}{2}(|0^n\rangle + i^{k_1}|s_1\rangle + i^{k_2}|s_2\rangle + i^{k_3}|s_3\rangle)$ for some distinct computational basis states $|s_1\rangle, |s_2\rangle, |s_3\rangle$ and some integers k_1, k_2, k_3, so $|\psi_3\rangle$ similarly is a stabilizer state and satisfies $\langle \psi_2 | \psi_3\rangle = \langle \psi_3 | \psi_1\rangle = -\frac{1}{2}$. $\square$

C. Inner product algorithm

We now turn our attention to computing inner products between extended graph states. Our inner product algorithm has cubic worst case runtime, same as the current best algorithm, based on generator matrices [3]. Our algorithm is more direct in implementation due to the correspondence between an extended graph state and the gates required to produce it and is also naturally global phase sensitive. Our algorithm uses the following observation.

Proposition V.10. *Let $|\psi\rangle \equiv \bigotimes_{i=1}^{n} c_i z_i |G\rangle$ be in reduced form, and let $A \equiv \{i | c_i = H\}$. Then*

$$\langle 0|^{\otimes n} |\psi\rangle = \begin{cases} 0 & \exists i \in A, z_i = Z \\ \frac{1}{\sqrt{2^{n-|A|}}} & \textit{otherwise} \end{cases} . \tag{25}$$

Proof. Note that

$$\langle 0|^{\otimes n} \bigotimes_{i=1}^{n} c_i z_i |G\rangle = \langle 0|^{\otimes n} \prod_{p\in A} H_p (z_p)_p |+\rangle^{\otimes n} = \frac{1}{\sqrt{2^{n-|A|}}} \langle 0|_A \prod_{p\in A} (x_p)_p |0\rangle^{\otimes n},$$

where $x_p = X$ when $z_p = Z$ and $x_p = I$ when $z_p = I$. If $x_p = X$ for some $p \in A$, then $\langle 0|^{\otimes n} |\psi\rangle = 0$ and otherwise $\langle 0|^{\otimes n} |\psi\rangle = \frac{1}{\sqrt{2^{n-|A|}}}$. □

We present our algorithm in the proof of the following theorem.

Theorem V.11. *Let* $|\psi\rangle \equiv \bigotimes_{i=1}^{n} C_i |G\rangle$ *and* $|\psi'\rangle \equiv \bigotimes_{i=1}^{n} C'_i |G'\rangle$ *be two extended graph states. Then* $\langle\psi|\psi'\rangle$ *can be computed in* $O(nd^2)$ *time, where* d *is the maximum degree in* G *and* G' *encountered during the calculation.*

Proof. First we apply $C_i^\dagger$ to C'_i for each i. It suffices to take the inner product of $|G\rangle$ and $\bigotimes_{i=1}^{n} D_i |G'\rangle$ for local Clifford operators D_i. We do so by taking the inner product of $|0\rangle^{\otimes n}$ and $|\varphi\rangle \equiv \bigotimes_{i=1}^{n} H \prod_{(i,j)\in E(G)} CZ_{i,j} \bigotimes_{i=1}^{n} D_i |G\rangle$. We first simplify the layer of CZ operators.

Definition V.12. A *star operation* on qubit p is a product of CZ operators, each having one of the qubits it is applied to equal p.

For each $p \in [n]$, we apply star operations of the form $\prod_{q\in N(p), q>p} CZ_{p,q}$ to $\bigotimes_{i=1}^{n} D_i |G'\rangle$. We perform updates in $O(d^2)$ time as follows. If D_p takes Z to $\pm Z$ upon conjugation, then for each neighbor q of p we apply $CZ_{p,q}$ by the method described in Section IV, conjugating it through D_p and D_q and either applying a normal CZ gate to G', Lemma C.1, or Lemma C.2. After updating D_i and G', D_p still takes Z to $\pm Z$ upon conjugation since D_p is changed by a diagonal Clifford, so we can repeat the same update process for all qubits q. If D_p takes Z to $\pm X$ upon conjugation, we apply Theorem III.11 to qubit p and some neighbor q of p, which changes D_p to $D_p H$. We proceed as before because D_p now takes Z to $\pm Z$ upon conjugation. If qubit p does not have a neighbor, then the application of the X operator to qubit p does not change $|G'\rangle$, so applying $CZ_{p,q}$ becomes equivalent to applying some Pauli operator on qubit q, which is trivial. If D_p takes Z to $\pm Y$ upon conjugation, then we apply Theorem III.10 to qubit p, which changes D_p to $D_p H S^\dagger H$. We proceed as in the first case because D_p takes Z to $\pm Z$.

Next, we append H to D_i for all i and simplify $\bigotimes_{i=1}^{n} D_i |G'\rangle$ to reduced form, following the algorithm described in Theorem III.12. $\langle\psi|\psi'\rangle$ is equal to the product of the result of Proposition V.10 applied to $|\varphi\rangle$ and the global phase factors produced during the calculation. The total runtime of the algorithm is $O(nd^2)$. □

VI. CONCLUSIONS

In this paper, we explored the stabilizer formalism through the lens of the graph formalism. We created a canonical form for expressing extended graph states in a concise and unique way that improves upon previous reduced forms [1, 19, 20]. We developed efficient simplification and inner product algorithms, and the connections between stablizer states and the properties of their corresponding graphs when expressed in canonical form can be explored in future work.

We applied our merging formulas to discover new rules that describe the action of controlled-Z gates on arbitrary extended graph states. Our transformation rules enable us to simplify GraphSim's algorithm for applying controlled-Pauli operators to graph states [7, 14] and improve runtime. We apply our transformation rules to prove that under certain assumptions, it is impossible to update extended graph states in under quadratic time in the number of qubits upon the application of a controlled-Pauli gate. Therefore, in order to improve graph state simulation, we should consider algorithms that do not simply apply one gate at a time. Whenever multiple CZ gates can be applied consecutively, we can potentially apply star operations following the method described in the proof of Theorem V.11 to spread out the $O(d^2)$ update time over multiple CZ gates, improving performance. Future work to improve graph state simulation could study the relationship between the circuit and the runtime, as well as design more efficient algorithms for simulating certain types of circuits, both those that graph state simulation is already suitable for, such as quantum error-correcting circuits, or other circuits.

We improved upon previous results [2, 21] by deriving a simpler graph merging formula and by completely characterizing linearly dependent triplets of stabilizer states. Both our characterization in terms of extended graph states and in terms of inner products reveal much structure in the additive properties of stabilizer states that can possibly be generalized. Future work can continue characterizing linearly dependent n-tuples of stabilizer states for $n \geq 4$ as well as stabilizer decompositions of magic states [6, 8–10], using the graph formalism. The appendices are organized as follows. Appendix A contains proofs of Theorems III.11 and V.3, Appendix B contains a discussion of improving upper bounds on the stabilizer rank of magic states, and Appendix C contains proofs for our graph state transformation rules.

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VII. APPENDICES

Appendix A: Proofs of Theorems III.11 and V.3

Here we prove Theorem III.11.

Proof. Without loss of generality let $x = 1$ and $y = 2$, $b_1, b_2 \in \{0,1\}$, and s be some binary string of length $n-2$. It suffices to show

$$\Big(\langle b_1 b_2| \otimes \langle s|\Big) H_x H_y |G\rangle = \Big(\langle b_1 b_2| \otimes \langle s|\Big) Z_x Z_y \prod_{p\in A, q\in B} CZ_{p,q} |G\rangle .$$

Let s_i denote the bit in s corresponding to qubit i, where $3 \le i \le n$. Let $a \equiv |\{p \in A \setminus B | s_p = 1\}|$, $b \equiv |\{p \in A \cap B \setminus \{1,2\} | s_p = 1\}|$, $c \equiv |\{p \in B \setminus A | s_p = 1\}|$. Then, the left hand side can be evaluated in terms of a, b, c as follows:

$$\begin{aligned}
&\Big(\langle b_1 b_2| \otimes \langle z|\Big) H_1 H_2 |G\rangle \\
&= \frac{1}{2} \sum_{(j,k)\in\{0,1\}^2} (-1)^{b_1 j + b_2 k} \Big(\langle jk| \otimes \langle z|\Big) |G\rangle \\
&= \frac{1}{2} \sum_{(j,k)\in\{0,1\}^2} (-1)^{b_1 j + b_2 k + j(a+b) + k(b+c) + jk} \\
&\qquad \cdot \Big(\langle 00| \otimes \langle z|\Big) |G\rangle ,
\end{aligned}$$

while for the right hand side, letting $A' \equiv A\setminus\{1,2\}$, $B' \equiv B \setminus \{1,2\}$,

$$\begin{aligned}
&\Big(\langle b_1 b_2| \otimes \langle z|\Big) Z_x Z_y \prod_{p\in A, q\in B} |G\rangle \\
&= \Big(\langle b_1 b_2| \otimes \langle z|\Big) \prod_{p\in A'} CZ_{p,1} CZ_{p,2} \\
&\quad \cdot \prod_{q\in B'} CZ_{1,q} CZ_{2,q} \prod_{p\in A', q\in B'} CZ_{p,q} |G\rangle \\
&= (-1)^{b_1(a+c)+b_2(a+c)+ab+bc+ca+b} \Big(\langle b_1 b_2| \otimes \langle z|\Big) |G\rangle \\
&= (-1)^{\zeta} \Big(\langle 00| \otimes \langle z|\Big) |G\rangle ,
\end{aligned}$$

where $\zeta = b_1(a+c) + b_2(a+c) + ab + bc + ca + b + b_1(a+b) + b_2(b+c) + b_1 b_2$. It suffices to verify

$$\frac{1}{2} \sum_{(j,k)\in\{0,1\}^2} (-1)^{b_1 j + b_2 k + j(a+b) + k(b+c) + jk} = (-1)^{\zeta}$$

for all $(a, b, c, b_1, b_2) \in \{0,1\}^5$. □

Here we prove Theorem V.3.

Proof. Without loss of generality let $x = 1$ and $y = 2$, $b_1, b_2 \in \{0,1\}$, and s be some binary string of length $n-2$. It suffices to show

$$\begin{aligned}
\Big(\langle b_1 b_2| \otimes \langle s|\Big) H_x H_y |G\rangle &= \Big(\langle b_1 b_2| \otimes \langle s|\Big) Z_x Z_y |G\rangle \\
&+ \Big(\langle b_1 b_2| \otimes \langle s|\Big) \prod_{p\in A, q\in B} CZ_{p,q} |G\rangle . \quad \text{(A1)}
\end{aligned}$$

Let s_i denote the bit in s corresponding to qubit i, where $3 \le i \le n$. Let $a \equiv |\{p \in A \setminus (B \cup \{1\}) | s_p = 1\}|$, $b \equiv |\{p \in A \cap B | s_p = 1\}|$, and $c \equiv |\{p \in B \setminus (A \cup \{1\}) | s_p = 1\}|$. Then, the left hand side can be evaluated in terms of a, b, c similarly as in the proof of Theorem III.11:

$$\begin{aligned}
&\Big(\langle b_1 b_2| \otimes \langle s|\Big) H_x H_y |G\rangle = \frac{1}{2} \\
&\cdot \sum_{(j,k)\in\{0,1\}^2} (-1)^{b_1 j + b_2 k + j(a+b) + k(b+c)} \Big(\langle 00| \otimes \langle z|\Big) |G\rangle .
\end{aligned}$$

The first term in the right hand side of Equation A1 is

$$\begin{aligned}
&\Big(\langle b_1 b_2| \otimes \langle s|\Big) Z_x Z_y |G\rangle = (-1)^{b_1 + b_2} \Big(\langle b_1 b_2| \otimes \langle s|\Big) \\
&\quad \cdot |G\rangle = (-1)^{b_1 + b_2 + b_1(a+b) + b_2(b+c)} \Big(\langle 00| \otimes \langle s|\Big) |G\rangle ,
\end{aligned}$$

while the second term in the right hand side is

$$\begin{aligned}&\Big(\langle b_1 b_2| \otimes \langle s|\Big) \prod_{p\in \mathrm{N}(x)} Z_p \prod_{q\in \mathrm{N}(y)} Z_q \prod_{p\in A, q\in B} CZ_{p,q} |G\rangle \\ &= (-1)^{a+c}\Big(\langle b_1 b_2| \otimes \langle s|\Big) CZ_{1,2} \\ &\cdot \prod_{p\in A} CZ_{p,2} \prod_{q\in B} CZ_{1,q} \prod_{p\in \mathrm{N}(1), q\in \mathrm{N}(2)} CZ_{p,q} |G\rangle \\ &= (-1)^{a+c+b_1b_2+b_1(b+c)+b_2(a+b)+ab+bc+ca+b} \\ &\cdot \Big(\langle b_1 b_2| \otimes \langle s|\Big) |G\rangle \\ &= (-1)^{a+b+c+b_1b_2+(b_1+b_2)(a+c)+ab+bc+ca} \\ &\cdot \Big(\langle 00| \otimes \langle s|\Big) |G\rangle .\end{aligned}$$

It suffices to verify

$$\begin{aligned}&\frac{1}{2}\sum_{(j,k)\in\{0,1\}^2} (-1)^{b_1 j + b_2 k + j(a+b) + k(b+c)} \\ &= (-1)^{b_1+b_2+b_1(a+b)+b_2(b+c)} \\ &+ (-1)^{a+c+b_1b_2+b_1(a+c)+b_2(a+c)+ab+bc+ca+b}\end{aligned}$$

for all $(a,b,c,b_1,b_2) \in \{0,1\}^5$. □

Appendix B: Stabilizer rank of magic states

Here we discuss our attempts at finding upper bounds on the stabilizer rank of n-qubit magic states, which we first define.

Definition B.1. A *n-qubit magic state* $|T_n\rangle$ is the state $|T\rangle^{\otimes n}$, where $|T\rangle \equiv \frac{|0\rangle + e^{\frac{\pi i}{4}}|1\rangle}{\sqrt{2}}$.

Definition B.2. The *stabilizer rank* $\chi(|\psi\rangle)$ of a state $|\psi\rangle$ is the smallest integer χ such that there exists a set of χ stabilizer states S such that $|\psi\rangle \in \mathrm{span}(S)$.

The stabilizer rank of the magic state is deeply tied to the runtimes of classical simulations of quantum circuits and has been explored extensively [8–10]. In order to tighten the upper bounds on $\chi(|T_n\rangle)$, a Metropolis-Hastings numerical search algorithm that applies random transformations to stabilizer states to maximize the projection of the magic state onto their span was developed [10]. We experimented with different variations of this method and were unable to find stabilizer decompositions for higher numbers of qubits, due to the extremely large search space. Another method, introduced in [6], utilizes *cat states* and *contractions*. It produced the best known upper bounds on $\chi(|T_n\rangle)$ by enabling a 6 qubit decomposition of the 6 qubit magic state to be found by inspection. However, for higher qubit states, inspection cannot be used and computing stabilizer decompositions once again becomes difficult.

Therefore, we tried a new method, which was to represent the n qubit magic state, $(T|+\rangle)^{\otimes n}$, as a linear combination of extended graph states written in our canonical form. By comparing pairs of extended graph states, we can see whether they can be merged together. We were able to use Mathematica to express the n qubit magic state as a sum of $2^{\frac{n}{2}}$ stabilizer states. At this point, though, we were not able to apply any more merges. Future work could try to develop more general merging criteria and formulas involving more than three extended graph states. Then, a computer could continually transform the sum of extended graph states following some sort of heuristic that allows it to stumble upon an optimal decomposition with some luck. In order to find such a heuristic, it would be useful to study properties of sums of extended graph states that provide more insights into the structure of low-rank stabilizer decompositions. So, we converted the stabilizer decompositions found in [6, 10] into our canonical form to see if we could glean any insights about their structure. We provide examples of stabilizer decompositions for two special cases, $n = 3$ and $n = 6$.

$$\begin{aligned}&(T|+\rangle)^{\otimes 3} = \frac{i - e^{i\frac{\pi}{4}}}{2} Z_1 Z_2 Z_3 |I_3\rangle \\ &- \frac{i + e^{\frac{\pi i}{4}}}{2} Z_1 Z_2 Z_3 |K_3\rangle + \frac{1 + e^{i\frac{\pi}{4}}}{2} H_1 H_2 S_3 |S_{3,3}\rangle \\ &(T|+\rangle)^{\otimes 6} = -\frac{\sqrt{i}}{2\sqrt{2}} H_6 (HZ)^{\otimes 6} |S_{6,6}\rangle \\ &+ \frac{1}{2\sqrt{2}} H^{\otimes 6} H_6 S_6 Z_6 |S_{6,6}\rangle - \frac{i}{2} H_1 S_1 S^{\otimes 6} |S_{6,1}\rangle \\ &+ \frac{i\sqrt{i}}{2} H_1 |S_{6,1}\rangle - \frac{1}{2} H_1 S_1 Z_1 (SZ)^{\otimes 6} |K_6\rangle \\ &- \frac{\sqrt{i}}{2} H_1 Z_1 Z^{\otimes 6} |K_6\rangle , \end{aligned} \tag{B1}$$

where $S_{n,i}$ is the star graph on n vertices with central vertex i. Even for the 3 qubit case, there are multiple ways to decompose the magic state into 3 stabilizer states, yet in all of the ways, there seems to be an empty graph, a complete graph, and a star graph. Future work can completely characterize the 3 qubit case and move on to higher cases.

Appendix C: Proofs of CZ transformation rules

Here we prove the expressions for $|\psi_{PQ}\rangle$ in Table I. $|\psi_{ZZ}\rangle$ is trivial.

Lemma C.1 (Elliot et al.)**.**

$$|\psi_{ZX}\rangle = \prod_{x\in N_2} CZ_{1,x} |G\rangle . \tag{C1}$$

Proof. Let G' be the graph formed from G where all the edges incident to 1 are removed. Suppose 1 is connected to 2 in G. Applying Theorem V.1, we have

$$\begin{aligned}
&\frac{1}{2}\left(\underbrace{(I+Z)_1\,|G\rangle}_{A=M_1,B=\{1\}} + X_2\underbrace{(I-Z)_1\,|G\rangle}_{A=M_1,B=\{1\}}\right)\\
&= \frac{1}{\sqrt{2}}H_1\,|G'\rangle + X_2\frac{1}{\sqrt{2}}H_1Z_1\left(\prod_{x\in N_1} Z_x\right)|G'\rangle\\
&= \frac{1}{\sqrt{2}}H_1\underbrace{\left(I - Z_1\prod_{x\in N_1} Z_x \prod_{x\in N_2\setminus\{1\}} Z_x\right)|G'\rangle}_{A=\{1\},B=N_1\triangle N_2}\\
&= \prod_{x\in N_1\triangle N_2} CZ_{1,x}\,|G'\rangle = \prod_{x\in N_2} CZ_{1,x}\,|G\rangle
\end{aligned}$$

Now suppose 1 is not connected to 2 in G. We have

$$\begin{aligned}
&\frac{1}{2}\left(\underbrace{(I+Z)_1\,|G\rangle}_{A=M_1,B=\{1\}} + X_2\underbrace{(I-Z)_1\,|G\rangle}_{A=M_1,B=\{1\}}\right)\\
&= \frac{1}{\sqrt{2}}H_1\,|G'\rangle + X_2\frac{1}{\sqrt{2}}H_1Z_1\left(\prod_{x\in N_1} Z_x\right)|G'\rangle\\
&= \frac{1}{\sqrt{2}}H_1\underbrace{\left(I + Z_1\prod_{x\in N_1} Z_x \prod_{x\in N_2} Z_x\right)|G'\rangle}_{A=\{1\},B=M_1\triangle N_2}\\
&= Z_1\prod_{x\in M_1\triangle N_2} CZ_{1,x}\,|G'\rangle = \prod_{x\in N_2} CZ_{1,x}\,|G\rangle
\end{aligned}$$

□

Lemma C.2.

$$|\psi_{YZ}\rangle = S_2Z_2\prod_{x\in M_1} CZ_{2,x}\,|G\rangle\,. \tag{C2}$$

Proof. Let G' refer to the graph resulting from toggling all the edges between vertices in the set M_1 in G. Applying Theorem V.2, we have

$$\begin{aligned}
&\frac{1}{2}\left(\underbrace{(I-iZ_1X_1)\,|G\rangle}_{A=M_1} + Z_2\underbrace{(I+iZ_1X_1)\,|G\rangle}_{A=M_1}\right)\\
&= \frac{1-i}{2}S_1\prod_{x\in N_1} S_x\,|G'\rangle + Z_2\frac{1+i}{2}S_1^3\prod_{x\in N_1} S_x^3\,|G'\rangle\\
&= \frac{1-i}{2}S_1\prod_{x\in N_1} S_x\underbrace{\left(I + iZ_2\prod_{x\in N_1} Z_x\right)|G'\rangle}_{A=M_1\triangle\{2\}}\\
&= S_1\prod_{x\in N_1} S_x \prod_{x\in M_1\triangle\{2\}} S_x^3 \prod_{x\in M_1\setminus\{2\}} CZ_{2,x}\,|G\rangle\\
&= S_2Z_2\prod_{x\in M_1} CZ_{2,x}\,|G\rangle
\end{aligned}$$

where the final step can be seen from case work on whether $2\in N_1$. □

Lemma C.3 (Elliot et al.)**.** *If* $(1,2)\in E(G)$,

$$|\psi_{XX}\rangle = H_1H_2CZ_{1,2}\prod_{x\in M_1,y\in M_2} CZ_{x,y}\,|G\rangle\,. \tag{C3}$$

Otherwise,

$$|\psi_{XX}\rangle = \prod_{x\in N_1,y\in N_2} CZ_{x,y}\,|G\rangle\,. \tag{C4}$$

Proof. If 1 and 2 are connected in G, we apply Theorem III.11

$$\begin{aligned}
|\psi_{XX}\rangle &= H_1H_2CZ_{1,2}H_1H_2\,|G\rangle\\
&= H_1H_2CZ_{1,2}\prod_{x\in M_1,y\in M_2} CZ_{x,y}\,|G\rangle
\end{aligned}$$

If 1 and 2 are not connected we follow the proof given in [19]. □

Lemma C.4. *If* $(1,2)\in E(G)$,

$$|\psi_{YX}\rangle = \frac{1-i}{\sqrt{2}}\left(\prod_{x\in M_1} S_x\right)H_1\prod_{x\in M_1\triangle M_2} CZ_{1,x}\,|L_1(G)\rangle\,. \tag{C5}$$

Otherwise,

$$|\psi_{YX}\rangle = \prod_{x\in M_1\triangle N_2} Z_x \prod_{x,y\in M_1\triangle N_2} CS_{x,y}\prod_{x,y\in M_1} CS_{x,y}\,|G\rangle\,. \tag{C6}$$

Proof. Let G' be G with all edges between vertices in M_1

toggled. If vertices 1 and 2 are connected in G,

$$\frac{1}{2}\left(\underbrace{(I-iZ_1X_1)\left|G\right\rangle}_{A=M_1}+X_2\underbrace{(I+iZ_1X_1)\left|G\right\rangle}_{A=M_1}\right)$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\left|G'\right\rangle+Y_2\frac{1+i}{2}\prod_{x\in M_1}S_x^3\left|G'\right\rangle$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\left|G_1\right\rangle+(1+i)\prod_{x\in M_1}S_x^3Y_2\left|G'\right\rangle$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\underbrace{\left(I+Z_2\prod_{x\in M_1}Z_x\prod_{x\in M_2\triangle M_1}Z_x\right)\left|G'\right\rangle}_{A=\{1\},B=N_2}$$
$$=\frac{1-i}{\sqrt{2}}\left(\prod_{x\in M_1}S_x\right)H_1\prod_{x\in N_2}CZ_{1,x}\left|G'\right\rangle$$
$$=\frac{1-i}{\sqrt{2}}\left(\prod_{x\in M_1}S_x\right)H_1\prod_{x\in N_1\cup N_2}CZ_{1,x}\left|L_1(G)\right\rangle$$

If vertices 1 and 2 are not connected in G,

$$\frac{1}{2}\left(\underbrace{(I-iZ_1X_1)\left|G\right\rangle}_{A=M_1}+X_2\underbrace{(I+iZ_1X_1)\left|G\right\rangle}_{A=M_1}\right)$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\left|G'\right\rangle+X_2\frac{1+i}{2}\prod_{x\in M_1}S_x^3\left|G'\right\rangle$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\underbrace{\left(I+iZ_2\prod_{x\in M_1}Z_x\prod_{x\in M_2}Z_x\right)\left|G'\right\rangle}_{A=M_1\triangle N_2}$$
$$=\prod_{x\in N_1}S_x\prod_{x\in M_1\triangle N_2}Z_x\prod_{x,y\in M_1\triangle N_2}CS_{x,y}\left|G'\right\rangle$$
$$=\prod_{x\in M_1\triangle N_2}Z_x\prod_{x,y\in M_1\triangle N_2}CS_{x,y}\prod_{x,y\in M_1}CS_{x,y}\left|G\right\rangle$$

□

Lemma C.5. *If* $(1,2)\in E(G)$,

$$\left|\psi_{YY}\right\rangle \;=\; -i\prod_{x,y\in M_1}CS_{x,y}\prod_{x,y\in M_2}CS_{x,y}\left|G\right\rangle. \quad \text{(C7)}$$

Otherwise,

$$\left|\psi_{YY}\right\rangle=\frac{1-i}{\sqrt{2}}\prod_{x\in M_1}S_xH_1\prod_{x\in M_2}CZ_{1,x}\left|L_1(G)\right\rangle. \quad \text{(C8)}$$

Proof. Let G' be G with all edges between vertices in M_1 toggled. If vertices 1 and 2 are connected in G,

$$\frac{1}{2}\left(\underbrace{(I-iZ_1X_1)\left|G\right\rangle}_{A=M_1}+Y_2\underbrace{(I+iZ_1X_1)\left|G\right\rangle}_{A=M_1}\right)$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\left|G'\right\rangle+Y_2\frac{1+i}{2}\prod_{x\in M_1}S_x^3\left|G'\right\rangle$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\left|G'\right\rangle-(1+i)\prod_{x\in M_1}S_x^3X_2\left|G'\right\rangle$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\left(I-i\prod_{x\in M_1}Z_x\prod_{x\in M_2\triangle M_1}Z_x\right)\left|G'\right\rangle$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\underbrace{\left(I-i\prod_{x\in M_2}Z_x\right)\left|G'\right\rangle}_{A=M_2}$$
$$=-i\prod_{x\in M_1}S_x\prod_{x,y\in M_2}CS_{x,y}\left|G'\right\rangle$$
$$=-i\prod_{x,y\in M_1}CS_{x,y}\prod_{x,y\in M_2}CS_{x,y}\left|G\right\rangle$$

If vertices 1 and 2 are not connected in G,

$$\frac{1}{2}\left(\underbrace{(I-iZ_1X_1)\left|G\right\rangle}_{A=M_1}+Y_2\underbrace{(I+iZ_1X_1)\left|G\right\rangle}_{A=M_1}\right)$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\left|G'\right\rangle+Y_2\frac{1+i}{2}\prod_{x\in M_1}S_x^3\left|G'\right\rangle$$
$$=\frac{1-i}{2}\prod_{x\in M_1}S_x\underbrace{\left(I+\prod_{x\in M_1}Z_x\prod_{x\in M_2}Z_x\right)\left|G'\right\rangle}_{A=\{1\},B=M_1\triangle M_2}$$
$$=\frac{1-i}{\sqrt{2}}\prod_{x\in M_1}S_xH_1Z_1\prod_{x\in M_1\triangle M_2}CZ_{1,x}\left|G'\right\rangle$$
$$=\frac{1-i}{\sqrt{2}}\prod_{x\in M_1}S_xH_1\prod_{x\in M_2}CZ_{1,x}\left|L_1(G)\right\rangle$$

□

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