

A graph theoretical approach to states and unitary operations

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Abstract Building upon our previous work, on graphical representation of a quantum state by signless Laplacian matrix, we pose the following question. If a local unitary operation is applied to a quantum state, represented by a signless Laplacian matrix, what would be the corresponding graph and how does one implement local unitary transformations graphically? We answer this question by developing the notion of local unitary equivalent graphs. We illustrate our method by a few, well known, local unitary transformations implemented by single qubit Pauli and Hadamard gates. We also show how graph switching can be used to implement the action of the C_{NOT} gate, resulting in a graphical description of Bell state generation.

Keywords Signless Laplacian of a combinatorial graph · Graph switching · Pauli matrices · Local unitary operators

1 Introduction

Humans are fundamentally visual beings. Our most intuitive senses are geometric and topological. Thus having a sense for graphs comes naturally to us. On the other extreme, perhaps the subtlest concept in physics, farthest

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removed from our sensory intuition, is the nature of quantum superposition, which asserts that particle properties may lack a definiteness or realism in a profoundly fundamental sense. Thus it is worthwhile asking how we may leverage the lucidity of the graphs to represent quantum states. A graph theoretical approach to quantum mechanics would also help to amalgamate visualization offered by graphs with the well developed mathematical machinery of graph theory. This motivated us to provide a graphical representation of quantum states in [1], where we showed that the concept of a signless Laplacian matrix is more advantageous, for graphical representation of quantum states, than the combinatorial Laplacian matrix.

Here we build upon our previous construction, of representing quantum states by density matrices defined by using signless Laplacian matrices associated with weighted graphs without multiple edges and with/without loops. Our main intention is to establish a proof of principle, and study the graph theoretic transformation associated with the simplest non-trivial operation on n qubits, namely the local unitary transformation of n qubits. This would have direct relevance to the field of quantum information [[2] ... [10]] which has been brought to the realms of practical endeavours by mean of spectacular experimental advances, such as in [11], [12].

If G is a weighted graph with/without loops having real edge weights and nonnegative loop weights, the density matrix defined by G is

$$\rho(G) = \frac{1}{\text{tr}(L(G))} L(G)$$

where $L(G)$ is the signless Laplacian matrix associated with the graph G , see [1]. Some of the well known unitary transformations are implemented by the Pauli $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ and $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ operators or their combination $H = \frac{X+Z}{\sqrt{2}}$, the Hadamard operator. These operations are also synonymous with the corresponding single-qubit logic gates. Another well known two-qubit operation is realized by the so called C_{NOT} gate, which together with suitable combinations of single-qubit gates can be shown to be adequate for universal quantum computation [13].

In this paper, we restrict our attention to weighted undirected graphs of order 2^n for any natural number n . We introduce new graph theoretic operations or switching methods for weighted graphs by using quantum logic gates (for example, Pauli matrices) on single qubits which produce cospectral and signless Laplacian cospectral weighted undirected graphs. By (signless Laplacian) cospectral we imply two graphs with equal multi-set of eigenvalues of the corresponding (signless Laplacian) adjacency matrices.

Given a graph G of order 2^n we generate new graphs G^{U_k} by applying switching methods on G such that $\rho(G^{U_k}) = U_k \rho(G) U_k^\dagger$ for some unitary matrix U_k of the form

$$U_k = U^{(1)} \otimes \dots \otimes U^{(k-1)} \otimes U \otimes U^{(k+1)} \otimes \dots \otimes U^{(n)} \quad (1)$$

where $U \in \{X, Y, Z, H\}$ and $U^{(j)} = I_2$ the identity matrix of order 2 when $j \neq k$, and $k = 1, 2, \dots, n$.

It is evident that the unitary matrix U_k of order 2^n given in (1) is a local unitary transformation acting on the Hilbert space $\mathbb{C}^{2^{\otimes n}} \equiv \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_n$ where $\mathcal{H}_j = \mathbb{C}^2$ for $j = 1, 2, \dots, n$. Thus, we show that local unitary operations defined in (1) when applied on density matrix of a n -qubit quantum state $\rho(G)$ obtained by signless Laplacian matrix associated with a weighted graph G , can be realized by suitable graph switchings of the graph G . We call the switching equivalent graphs G and G^{U_k} the local unitary equivalent graphs.

The plan of the paper is as follows. In Section 2 we briefly review the connection between the concepts of graphs, quantum states, graph switching and local unitary operations. Next, we introduce graph switching methods which can realize local unitary operations applied to a density matrix associated with graphs. Thus we provide switching methods to generate cospectral and signless Laplacian cospectral weighted undirected graphs. *CNOT* gates are two qubit gates that, along with the single qubit Hadamard gate, are used to generate the two qubit maximally entangled Bell states. In Section 5 we show how the graph switching techniques can be used to implement the action of a *CNOT* gate, resulting in the graphical description of Bell state generation. We then make our conclusions.

2 Some Preliminaries

A graph $G = (V(G), E(G))$ is a combination of vertex set $V(G)$ and edge set $E(G)$. G is weighted if there is a weight function $w : E(G) \rightarrow \mathbb{R}$, $w(i, j) = w_{i,j}$. Adjacency matrix of G is $A(G) = (a_{i,j})$, where,

$$a_{i,j} = \begin{cases} w_{i,j} & \text{if } (i, j) \in E(G) \\ 0 & \text{if } (i, j) \notin E(G) \end{cases}.$$

Adjacency matrix represents connections between different vertices in a graph. Degree of vertex i is $d_i = \sum_j |a_{i,j}|$, and is indicative of the role played by the vertex i in the graph G . Degree matrix of G is $D(G) = \text{diag}\{d_i : i = 1, 2, \dots\}$. Originally, combinatorial Laplacian $\mathcal{L} = D(G) - A(G)$ was used for representing density matrices corresponding to quantum states [14, 15].

In [1], density matrices were constructed using signless and signed Laplacians. Here, our constructions are made using the signless Laplacian. In [16], it was shown that the signless Laplacian is most convenient for use in the study of the properties of graphs compared to any other matrix associated with a graph (generalized adjacency matrices). In [17], the authors have obtained an ensemble of density matrices as the normalized version of the signless Laplacian matrices which arise from a uniform mixture of unsigned edge-states in a simple graph.

For a weighted undirected graph G without multiple edges, with/without loops having real edge weights and nonnegative loop weights, the density matrix associated with $G = (V(G), E(G))$ is given by

$$\rho(G) = \frac{1}{\text{tr}(L(G))} L(G), \quad L(G) = D(G) + A(G) \quad (2)$$

The matrix $L(G)$ of order $|V(G)|$ is called the signless Laplacian matrix associated with G [1]. To normalize the state associated with $L(G)$, we divide it by its trace. If G has no loop, then $\text{trace}(D(G)) = \text{trace}(L(G))$. But here, $\text{trace}(D(G)) \neq \text{trace}(L(G))$ as graphs with weighted loops are considered. Hence, $\rho(G)$ is a Hermitian positive semi-definite matrix of trace 1 and hence represents the density matrix of a quantum state in $\mathbb{C}^{|V(G)|}$. The graph G is called a graph representation of $\rho(G)$. As an example consider $\rho_0 = |0\rangle\langle 0| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ and $\rho_1 = |1\rangle\langle 1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$. Graphs corresponding to ρ_0 and ρ_1 are



and

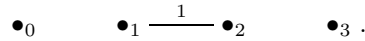


respectively. These graphs do not have any edge but have a loop of weight $\frac{1}{2}$.

The following observations can be proved by using arguments similar to those in [1].

- The density matrix defined by an undirected weighted graph G without loops of order n represents a pure state if and only if G is isomorphic to $\hat{K}_2 = K_2 \sqcup i_1 \sqcup \dots \sqcup i_{n-2}$, where K_2 is the complete graph of order 2 (a graph with two vertices and one weighted edge).
- The density matrix defined by an undirected weighted graph G with non-negative weighted loops of order n represents a pure state if and only if G is isomorphic to $\hat{O}_1 = O_1 \sqcup i_1 \sqcup i_2 \dots \sqcup i_{n-1}$, where O_1 denotes a graph having one node with self-loop.

As an example consider the graph in the figure below representing a well known two qubit pure quantum state $\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ [1], the Bell state.



A single qubit mixed state $a|0\rangle\langle 0| + b|1\rangle\langle 1|$, $a + b = 1$ can be represented by



Thus, the density matrix which represents an n -qubit multipartite quantum state defined by signless Laplacian matrix associated with an undirected weighted graph G of order 2^n with/without loops is a pure state if and only

if G contains only one edge. Otherwise, the density matrix $\rho(G)$ represents a mixed state.

Switching of a weighted graph G is a technique to generate a new weighted graph H from G keeping the vertex set fixed. Thus, switching a graph $G = (V(G), E(G))$ means constructing a graph $H = (V(H), E(H))$ such that

- $V(H) = V(G)$.
- $E(H)$ is given by $E(G)$ after removing/adding some weighted edges and/or altering weights of the edges in G .

The graphs G and H are called switching equivalent graphs. The switching method was first proposed in [18] for simple graphs that can produce cospectral simple graphs. Such a switching is well known as Seidel switching in the literature. Recently, some switching methods have been proposed in literature for directed, undirected and weighted graphs to generate cospectral, combinatorial Laplacian cospectral and signless Laplacian cospectral graphs [19], [20], respectively.

Familiar single qubit gates are X, Y, Z and H . They work on single qubit quantum states $|0\rangle, |1\rangle$ and there linear combinations. Graphically we can represent their actions on ρ_0 and ρ_1 as:

1. **X gate:** Note that $X\rho_0X^\dagger = \rho_1$ and $X\rho_1X^\dagger = \rho_0$. Thus applying X gate on ρ_0 is equivalent to removing loop of weight $\frac{1}{2}$ from node 0 and adding a loop of weight $\frac{1}{2}$ at node 1. Corresponding action will be observed for ρ_1 . The graph theoretical representations of these actions are illustrated below.

$$\frac{1}{2} \text{ loop at } \bullet_0 \quad \bullet_1 \xrightarrow{X} \bullet_0 \quad \bullet_1 \text{ loop } \frac{1}{2}$$

and

$$\bullet_0 \quad \bullet_1 \text{ loop } \frac{1}{2} \xrightarrow{X} \frac{1}{2} \text{ loop at } \bullet_0 \quad \bullet_1$$

2. **Y gate:** As $Y\rho_0Y^\dagger = \rho_1$ and $Y\rho_1Y^\dagger = \rho_0$ and its graphical representation is similar to that of X above.
3. **Z gate:** Here $Z\rho_0Z^\dagger = \rho_0$ and $Z\rho_1Z^\dagger = \rho_1$. Graphically its action are given by

$$\frac{1}{2} \text{ loop at } \bullet_0 \quad \bullet_1 \xrightarrow{Z} \frac{1}{2} \text{ loop at } \bullet_0 \quad \bullet_1$$

and

$$\bullet_0 \quad \bullet_1 \text{ loop } \frac{1}{2} \xrightarrow{Z} \bullet_0 \quad \bullet_1 \text{ loop } \frac{1}{2}$$

4. **H gate:** $H\rho_0H^\dagger = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, which is the density matrix corresponding to

a graph with two vertices. $H\rho_1H^\dagger = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$, corresponding to a graph with two vertices with an edge of weight -1. Thus applying H gate on ρ_0 or ρ_1 is tantamount to removing loops from the nodes and adding an edge between the two nodes. This can be represented graphically as:

$$\frac{1}{2} \text{ loop at } \bullet_0 \quad \bullet_1 \xrightarrow{H} \bullet_0 \text{ --- } 1 \text{ --- } \bullet_1$$

and

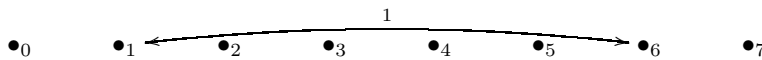
$$\bullet_0 \quad \bullet_1 \overset{\frac{1}{2}}{\curvearrowright} \xrightarrow{H} \bullet_0 \overset{-1}{\text{---}} \bullet_1 .$$

5. **CNOT gate:** *CNOT* is a two qubit gate whose matrix representation is denoted here by C_{NOT} .

$$C_{NOT} = \begin{bmatrix} I_2 & 0 \\ 0 & X \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} .$$

CNOT gate is useful for generating Bell states. Its graphical action on two qubit states is depicted at the end of section 5,

An n -qubit quantum state can be represented by a graph of order 2^n . As an example a 3-qubit quantum state $\frac{1}{\sqrt{2}}(|001\rangle + |110\rangle)$ can be represented as



Another, well known, example of a 3-qubit quantum state $|W\rangle = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle)$ can be represented [1] as



This graph corresponds to a state represented by a signed Laplacian, but here we do not make further use of this.

Action of local unitary operations on multi-partite systems have found place in the core of quantum information due to applications in several quantum information protocols. For example, quantum teleportation and quantum dense coding are based on the equivalence of some classes of states of bi-partite systems [6]. Since the entries of a density matrix representing a multi-partite quantum state depend on the choice of the basis in Hilbert space associated with the system, action of a local unitary operation implies change of the basis in the subsystems. Thus, a local unitary operation only changes our point of view without affecting the physical system.

Consider an n -qubit system given by the Hilbert space $\mathbb{C}^{2^{\otimes n}}$. Then two n -qubit states given by the density matrices ρ_1 and ρ_2 are said to be local unitary equivalent if there exists a unitary matrix U of order 2^n for which $\rho_2 = U\rho_1U^\dagger$ where U is of the form $U = U_1 \otimes U_2 \otimes \dots \otimes U_n$, U_i is a unitary matrix of order 2 for $i = 1, 2, \dots, n$.

In section 3, we develop switching methods for weighted undirected graphs such that for the two switching equivalent graphs G and G^{U_k} , $A(G^{U_k}) = U_k A(G) U_k^\dagger$ and

$$\rho(G^{U_k}) = U_k \rho(G) U_k^\dagger, U_k = U^{(1)} \otimes \dots \otimes U^{(k-1)} \otimes U \otimes U^{(k+1)} \otimes \dots \otimes U^{(n)},$$

where, $U \in \{X, Y, Z, H\}$ and $U^{(j)} = I_2$ the identity matrix of order 2 when $j \neq k$, and $k = 1, 2, \dots, n$. Thus, the switching methods proposed in this paper preserve both the spectra and signless Laplacian spectra. Thereby, we introduce the concept of local unitary equivalent graphs which are useful for the realization of local unitary operations on n -qubit quantum states, represented by weighted undirected graphs of order 2^n .

3 Switching methods and local unitary equivalent n -qubit quantum states

In order to interpret switching equivalent weighted undirected graphs as local unitary equivalent n -qubit quantum states which are represented by graphs, we consider a block representation of the adjacency matrix associated with such a graph. Thus, given a weighted undirected graph $G = (V(G), E(G))$ of order 2^n , we consider a partition of the vertex set $V(G) = \{0, 1, \dots, 2^n - 1\}$ given by

$$V(G) = \sqcup_{j=0}^{2^{n-1}-1} C_j$$

where $C_j = \{2j, 2j+1\}$, $j = 0, 1, \dots, 2^{n-1} - 1$. Then the the adjacency matrix of G is given by

$$A(G) = \begin{bmatrix} C_{0,0} & C_{0,1} & \dots & C_{0,(2^{n-1}-1)} \\ C_{1,0} & C_{1,1} & \dots & C_{1,(2^{n-1}-1)} \\ \vdots & \vdots & \vdots & \vdots \\ C_{(2^{n-1}-1),0} & C_{(2^{n-1}-1),1} & \dots & C_{(2^{n-1}-1),(2^{n-1}-1)} \end{bmatrix}_{2^n \times 2^n} \quad (3)$$

$$\text{where } C_{i,j} = \begin{bmatrix} w(2i, 2j)|_G & w(2i, 2j+1)|_G \\ w(2i+1, 2j)|_G & w(2i+1, 2j+1)|_G \end{bmatrix}_{2 \times 2}$$

$$\text{and } C_{i,i} = \begin{bmatrix} w(2i, 2i)|_G & w(2i, 2i+1)|_G \\ w(2i+1, 2i)|_G & w(2i+1, 2i+1)|_G \end{bmatrix}_{2 \times 2}.$$

Obviously, $C_{i,j} = C_{j,i}$. Note that $C_{i,i}$ is the adjacency matrix corresponding to a subgraph induced by the vertex subset C_i and $C_{i,j}$ provides the information of the existence of edges between C_i and C_j for all i, j .

First we propose switching methods which can realize the local unitary operations given by $U_n = \underbrace{I_2 \otimes I_2 \otimes \dots \otimes I_2}_{(n-1) \text{ times}} \otimes U$ where $U = \begin{bmatrix} e^{i\phi_1} \cos(\theta) & e^{i\phi_2} \sin(\theta) \\ -e^{-i\phi_2} \sin(\theta) & e^{-i\phi_1} \cos(\theta) \end{bmatrix}$.

Procedure 1 Given an weighted undirected graph $G = (V(G), E(G))$ we propose the following rule to generate a new graph $G^{U_n} = (V(G), E(G^{U_n}))$. Each step of this procedure will be applied on different edges or loops present in the original graph one by one. To generate the resultant graph if more than one weights are assigned during the process on a single edge or loop, ultimately, all the assigned weights will be added up cumulatively to produce the resultant weight for each edge or loop.

1. Assign the following edge weights inside every module C_i when $E(G)$ contains loops in it.
 - (a) Let $(2i, 2i) \in E(G)$, then
 - i. $(2i, 2i) \in E(G^{U_n})$,
 $w(2i, 2i)|_{G^{U_n}} = e^{2i\phi_1} \cos^2(\theta)w(2i, 2i)|_G$
 - ii. $(2i, 2i+1) \in E(G^{U_n})$,
 $w(2i, 2i+1)|_{G^{U_n}} = e^{i(\phi_1+\phi_2)} \cos(\theta) \sin(\theta)w(2i, 2i)|_G$
 - iii. $(2i+1, 2i) \in E(G^{U_n})$,
 $w(2i+1, 2i)|_{G^{U_n}} = -e^{i(\phi_1-\phi_2)} \sin(\theta) \cos(\theta)w(2i, 2i)|_G$
 - iv. $(2i+1, 2i+1) \in E(G^{U_n})$,
 $w(2i+1, 2i+1)|_{G^{U_n}} = -\sin^2(\theta)w(2i, 2i)|_G$
 - (b) Let $(2i+1, 2i+1) \in E(G)$, then
 - i. $(2i, 2i) \in E(G^{U_n})$,
 $w(2i, 2i)|_{G^{U_n}} = -\sin^2(\theta)w(2i+1, 2i+1)|_G$
 - ii. $(2i, 2i+1) \in E(G^{U_n})$,
 $w(2i, 2i+1)|_{G^{U_n}} = e^{-i(\phi_1-\phi_2)} \cos(\theta) \sin(\theta)w(2i+1, 2i+1)|_G$
 - iii. $(2i+1, 2i) \in E(G^{U_n})$,
 $w(2i+1, 2i)|_{G^{U_n}} = -e^{-i(\phi_1+\phi_2)} \sin(\theta) \cos(\theta)w(2i+1, 2i+1)|_G$
 - iv. $(2i+1, 2i+1) \in E(G^{U_n})$,
 $w(2i+1, 2i+1)|_{G^{U_n}} = e^{-2i\phi_1} \cos^2(\theta)w(2i+1, 2i+1)|_G$
2. Assign the following edge weights inside a module when there is an edge inside a module.
 - (a) Let $(2i, 2i+1) \in E(G)$, then
 - i. $(2i, 2i) \in E(G^{U_n})$,
 $w(2i, 2i)|_{G^{U_n}} = -e^{i(\phi_1-\phi_2)} \cos(\theta) \sin(\theta)w(2i, 2i+1)|_G$
 - ii. $(2i, 2i+1) \in E(G^{U_n})$,
 $w(2i, 2i+1)|_{G^{U_n}} = \cos^2(\theta)w(2i, 2i+1)|_G$
 - iii. $(2i+1, 2i) \in E(G^{U_n})$,
 $w(2i+1, 2i)|_{G^{U_n}} = -e^{-2i\phi_2} \sin^2(\theta)w(2i, 2i+1)|_G$
 - iv. $(2i+1, 2i+1) \in E(G^{U_n})$,
 $w(2i+1, 2i+1)|_{G^{U_n}} = -e^{-i(\phi_1+\phi_2)} \sin(\theta) \cos(\theta)w(2i, 2i+1)|_G$
 - (b) Let $(2i+1, 2i) \in E(G)$, then
 - i. $(2i, 2i) \in E(G^{U_n})$,
 $w(2i, 2i)|_{G^{U_n}} = e^{i(\phi_1+\phi_2)} \cos(\theta) \sin(\theta)w(2i+1, 2i)|_G$
 - ii. $(2i, 2i+1) \in E(G^{U_n})$,
 $w(2i, 2i+1)|_{G^{U_n}} = e^{2i\phi_2} \sin^2(\theta)w(2i+1, 2i)|_G$
 - iii. $(2i+1, 2i) \in E(G^{U_n})$,
 $w(2i+1, 2i)|_{G^{U_n}} = \cos^2(\theta)w(2i+1, 2i)|_G$

- iv. $(2i+1, 2i+1) \in E(G^{U_n})$,
 $w(2i+1, 2i+1)|_{G^{U_n}} = e^{-i(\phi_1-\phi_2)} \sin(\theta) \cos(\theta) w(2i+1, 2i)|_G$
3. Assign these edge weights when there are edges joining vertices of different modules.
- (a) Let $(2i, 2j) \in E(G)$, then
- i. $(2i, 2j) \in E(G^{U_n})$,
 $w(2i, 2j)|_{G^{U_n}} = e^{2i\phi_1} \cos^2(\theta) w(2i, 2j)|_G$
- ii. $(2i, 2j+1) \in E(G^{U_n})$,
 $w(2i, 2j+1)|_{G^{U_n}} = e^{i(\phi_1+\phi_2)} \cos(\theta) \sin(\theta) w(2i, 2j)|_G$
- iii. $(2i+1, 2j) \in E(G^{U_n})$,
 $w(2i+1, 2j)|_{G^{U_n}} = -e^{i(\phi_1-\phi_2)} \sin(\theta) \cos(\theta) w(2i, 2j)|_G$
- iv. $(2i+1, 2j+1) \in E(G^{U_n})$,
 $w(2i+1, 2j+1)|_{G^{U_n}} = -\sin^2(\theta) w(2i, 2j)|_G$
- (b) Let $(2i+1, 2j+1) \in E(G)$, then
- i. $(2i, 2j) \in E(G^{U_n})$,
 $w(2i, 2j)|_{G^{U_n}} = -\sin^2(\theta) w(2i+1, 2j+1)|_G$
- ii. $(2i, 2j+1) \in E(G^{U_n})$,
 $w(2i, 2j+1)|_{G^{U_n}} = e^{-i(\phi_1-\phi_2)} \cos(\theta) \sin(\theta) w(2i+1, 2j+1)|_G$
- iii. $(2i+1, 2j) \in E(G^{U_n})$,
 $w(2i+1, 2j)|_{G^{U_n}} = -e^{-i(\phi_1+\phi_2)} \sin(\theta) \cos(\theta) w(2i+1, 2j+1)|_G$
- iv. $(2i+1, 2j+1) \in E(G^{U_n})$,
 $w(2i+1, 2j+1)|_{G^{U_n}} = e^{-2i\phi_1} \cos^2(\theta) w(2i+1, 2j+1)|_G$
- (c) Let $(2i, 2j+1) \in E(G)$, then
- i. $(2i, 2j) \in E(G^{U_n})$,
 $w(2i, 2j)|_{G^{U_n}} = -e^{i(\phi_1-\phi_2)} \cos(\theta) \sin(\theta) w(2i, 2j+1)|_G$
- ii. $(2i, 2j+1) \in E(G^{U_n})$,
 $w(2i, 2j+1)|_{G^{U_n}} = \cos^2(\theta) w(2i, 2j+1)|_G$
- iii. $(2i+1, 2j) \in E(G^{U_n})$,
 $w(2i+1, 2j)|_{G^{U_n}} = -e^{-2i\phi_2} \sin^2(\theta) w(2i, 2j+1)|_G$
- iv. $(2i+1, 2j+1) \in E(G^{U_n})$,
 $w(2i+1, 2j+1)|_{G^{U_n}} = -e^{-i(\phi_1+\phi_2)} \sin(\theta) \cos(\theta) w(2i, 2j+1)|_G$
- (d) Let $(2i+1, 2j) \in E(G)$, then
- i. $(2i, 2j) \in E(G^{U_n})$,
 $w(2i, 2j)|_{G^{U_n}} = e^{i(\phi_1+\phi_2)} \cos(\theta) \sin(\theta) w(2i+1, 2j)|_G$
- ii. $(2i, 2j+1) \in E(G^{U_n})$,
 $w(2i, 2j+1)|_{G^{U_n}} = e^{2i\phi_2} \sin^2(\theta) w(2i+1, 2j)|_G$
- iii. $(2i+1, 2j) \in E(G^{U_n})$,
 $w(2i+1, 2j)|_{G^{U_n}} = \cos^2(\theta) w(2i+1, 2j)|_G$
- iv. $(2i+1, 2j+1) \in E(G^{U_n})$,
 $w(2i+1, 2j+1)|_{G^{U_n}} = e^{-i(\phi_1-\phi_2)} \sin(\theta) \cos(\theta) w(2i+1, 2j)|_G$

Then we have the following theorem.

Theorem 1 Let G be a weighted undirected graph of order 2^n . Then $\rho(G^{U_n}) = U_n \rho(G) U_n^\dagger$ where $U_n = \underbrace{I_2 \otimes I_2 \otimes \dots \otimes I_2}_{(n-1) \text{ times}} \otimes U$.

Proof Note that,

$$U_n = \text{diag}\{U, U, \dots, U\}_{2^n \times 2^n} \text{ and}$$

$$U_n A(G) U_n^\dagger = \begin{bmatrix} UC_0 U^\dagger & UC_{0,1} U^\dagger & \dots & UC_{0,(2^{n-1}-1)} U^\dagger \\ UC_{1,0} U^\dagger & UC_1 U^\dagger & \dots & UC_{1,(2^{n-1}-1)} U^\dagger \\ \vdots & \vdots & \vdots & \vdots \\ UC_{(2^{n-1}-1),0} U^\dagger & UC_{(2^{n-1}-1),1} U^\dagger & \dots & UC_{(2^{n-1}-1)} U^\dagger \end{bmatrix}.$$

Here, C_i and $C_{i,j}$ are either the matrices given below or their sum.

$$\begin{bmatrix} w & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ 0 & w \end{bmatrix}, \begin{bmatrix} 0 & w \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 \\ w & 0 \end{bmatrix}.$$

Remaining proof follows from the fact that

$$U \begin{bmatrix} w & 0 \\ 0 & 0 \end{bmatrix} U^\dagger = \begin{bmatrix} e^{2i\phi_1} w \cos[\theta]^2 & e^{i\phi_1+i\phi_2} w \cos[\theta] \sin[\theta] \\ -e^{i\phi_1-i\phi_2} w \cos[\theta] \sin[\theta] & -w \sin[\theta]^2 \end{bmatrix},$$

$$U \begin{bmatrix} 0 & 0 \\ 0 & w \end{bmatrix} U^\dagger = \begin{bmatrix} -w \sin[\theta]^2 & e^{-i\phi_1+i\phi_2} w \cos[\theta] \sin[\theta] \\ -e^{-i\phi_1-i\phi_2} w \cos[\theta] \sin[\theta] & e^{-2i\phi_1} w \cos[\theta]^2 \end{bmatrix},$$

$$U \begin{bmatrix} 0 & w \\ 0 & 0 \end{bmatrix} U^\dagger = \begin{bmatrix} -e^{i\phi_1-i\phi_2} w \cos[\theta] \sin[\theta] & w \cos[\theta]^2 \\ e^{-2i\phi_2} w \sin[\theta]^2 & -e^{-i\phi_1-i\phi_2} w \cos[\theta] \sin[\theta] \end{bmatrix},$$

$$U \begin{bmatrix} 0 & 0 \\ w & 0 \end{bmatrix} U^\dagger = \begin{bmatrix} e^{i\phi_1+i\phi_2} w \cos[\theta] \sin[\theta] & e^{2i\phi_2} w \sin[\theta]^2 \\ w \cos[\theta]^2 & e^{-i\phi_1+i\phi_2} w \cos[\theta] \sin[\theta] \end{bmatrix}.$$

Hence proved.

Here U is the most general unitary matrix of order 2, as given above. The well known single qubit matrices can be obtained from it as special cases. For $\theta = \frac{\pi}{2}, \phi_2 = \frac{\pi}{2}, U = iX$; for $\theta = \frac{\pi}{2}, \phi_2 = \frac{3\pi}{2}, U = Y$; for $\theta = 0, \phi_1 = \frac{\pi}{2}, U = iZ$ and for $\theta = \frac{\pi}{4}, \phi_1 = \frac{\pi}{2}, \phi_2 = \frac{\pi}{2}, U = iH$. The complex number i acts as a phase factor having no role in unitary operations. Thus, for example, given a weighted undirected graph $G = (V(G), E(G))$, a new graph $G^{X_n} = (V(G), E(G^{X_n}))$, corresponding to $X_n = \underbrace{I_2 \otimes I_2 \otimes \dots \otimes I_2}_{(n-1) \text{ times}} \otimes X$, would be generated according

to the following rules.

1. Interchange loop weights inside every module C_i

$$\begin{aligned} (2i, 2i) \in E(G) &\Rightarrow (2i+1, 2i+1) \in E(G^{X_n}), (2i, 2i) \notin E(G^{X_n}) \\ &w(2i+1, 2i+1)|_{G^{X_n}} = w(2i, 2i)|_G, \\ (2i+1, 2i+1) \in E(G) &\Rightarrow (2i, 2i) \in E(G^{X_n}), (2i+1, 2i+1) \notin E(G^{X_n}) \\ &w(2i, 2i)|_G = w(2i+1, 2i+1)|_{G^{X_n}}. \end{aligned} \tag{4}$$

2. Keep edge weights inside modules unchanged

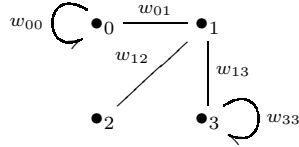
$$\begin{aligned} (2i, 2i+1) \in E(G) &\Rightarrow (2i, 2i+1) \in E(G^{X_n}) \\ w(2i, 2i+1)|_{G^{X_n}} &= w(2i, 2i+1)|_G. \end{aligned} \quad (5)$$

3. Modifications of edges joining two modules

$$\begin{aligned} (2i, 2j) \in E(G) &\Rightarrow (2i+1, 2j+1) \in E(G^{X_n}), (2i, 2j) \notin E(G^{X_n}) \\ w(2i+1, 2j+1)|_{G^{X_n}} &= w(2i, 2j)|_G, \\ (2i+1, 2j+1) \in E(G) &\Rightarrow (2i, 2j) \in E(G^{X_n}), (2i+1, 2j+1) \notin E(G^{X_n}) \\ w(2i, 2j)|_{G^{X_n}} &= w(2i+1, 2j+1)|_G, \\ (2i, 2j+1) \in E(G) &\Rightarrow (2j, 2i+1) \in E(G^{X_n}), (2i, 2j+1) \notin E(G^{X_n}) \\ w(2j, 2i+1)|_{G^{X_n}} &= w(2i, 2j+1)|_G, \\ (2j, 2i+1) \in E(G) &\Rightarrow (2i, 2j+1) \in E(G^{X_n}), (2j, 2i+1) \notin E(G^{X_n}) \\ w(2i, 2j+1)|_{G^{X_n}} &= w(2j, 2i+1)|_G. \end{aligned} \quad (6)$$

The following example provides an overview of the effect of local unitary operators X_n, Y_n, Z_n, H_n when applied to a 2-qubit density matrix of order 4, making use of the graph representations of the corresponding density matrix.

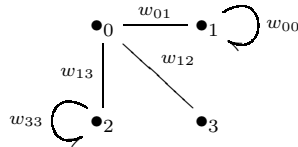
Example 1 Consider the graph,



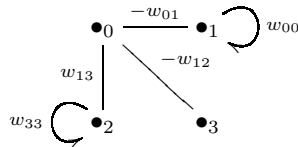
It represents following mixed two qubit state,

$$\rho = \frac{L(G)}{\text{tr}(L(G))} = \frac{1}{\text{tr}(L(G))} \begin{bmatrix} 2w_{00} + w_{01} & w_{01} & 0 & 0 \\ w_{01} & w_{01} + w_{12} + w_{13} & w_{12} & w_{13} \\ 0 & w_{12} & w_{12} & 0 \\ 0 & w_{13} & 0 & w_{13} + 2w_{33} \end{bmatrix},$$

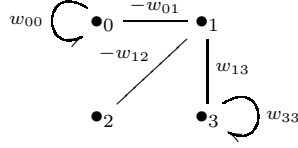
where $\text{tr}(L(G)) = 2(w_{00} + w_{01} + w_{12} + w_{13} + w_{33})$. Applying X_2 on the original graph:



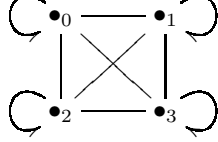
Applying Y_2 on the original graph:



Applying Z_2 on the original graph:



Applying H_2 on the original graph:



In this figure, the edge weights $w(i, j)$ where $(i, j) = 0, 1, 2, 3$ are

$$\begin{aligned}
 w(0, 1) &= w_{00} - \frac{1}{2}(w_{12} + w_{13}) \\
 w(0, 2) &= \frac{1}{2}w_{12} + \frac{1}{2}w_{13}, \\
 w(0, 3) &= \frac{1}{2}w_{12} - \frac{1}{2}w_{13}, \\
 w(1, 2) &= -\frac{1}{2}w_{12} - \frac{1}{2}w_{13}, \\
 w(1, 3) &= -\frac{1}{2}w_{12} + \frac{1}{2}w_{13}, \\
 w(2, 3) &= \frac{1}{2}w_{12} - \frac{1}{2}w_{13} - w_{33}, \\
 w(0, 0) &= w_{01} + \frac{w_{13}}{2}, \\
 w(1, 1) &= w_{12} + \frac{w_{13}}{2}, \\
 w(2, 2) &= w_{33} + \frac{w_{13}}{2}, \\
 w(3, 3) &= w_{33} + \frac{w_{13}}{2}.
 \end{aligned}$$

Thus the local unitary operators given by X_n, Y_n, Z_n and H_n acting on a density matrix $\rho(G)$ of an n -qubit quantum state defined by the signless Laplacian associated with a weighted undirected G can be realized by graph switchings applied on the graph G . Now we focus on the local unitary operators $U_k = I_2 \otimes \dots \otimes I_2 \otimes U \otimes I_2 \otimes \dots \otimes I_2$ when $k < n$ and $U \in \{X, Y, Z, H\}$ is placed in the k -th position of the tensor product.

In order to give a graph theoretic interpretation of U_k we represent the vertex set of a weighted undirected graph $G = (V(G), E(G))$ of order 2^n by $V(G) = \{0, 1\}^n \equiv \{0, 1, \dots, 2^n - 1\}$ where a vertex $j \in V(G)$ is represented by a sequence of 0, 1s. The labeling of the vertices of G is determined by the lexicographic ordering defined on $\{0, 1\}^n$. For example, if $n = 2$ the labeled vertex set is given by $V(G) = \{00, 01, 10, 11\} \equiv \{0, 1, 2, 3\}$.

We also consider a permutation $p_{k,n}$ on the vertex set $V(G)$ defined as follows

$$p_{k,n} : \{0, 1\}^n \rightarrow \{0, 1\}^n \quad (7)$$

$$x_1 x_2 \dots x_{k-1} x_k x_{k+1} \dots x_n \mapsto x_1 x_2 \dots x_{k-1} x_n x_{k+1} \dots x_k \quad (8)$$

where $x_i \in \{0, 1\}$. Thus given the standard lexicographic ordering on $\{0, 1\}^n$, $p_{k,n}$ introduces a relabeling of the vertices. Let $P_{k,n}$ be the unique permutation matrix associated with $p_{k,n}$. Then it is easy to verify that

$$A(G_{p_{k,n}}) = P_{k,n} A(G) P_{k,n}^\dagger, \quad D(G_{p_{k,n}}) = P_{k,n} D(G) P_{k,n}^\dagger \quad (9)$$

where $G_{p_{k,n}}$ denotes the graph G with a new labeling of the vertices given by $p_{k,n}$. Moreover, $U_k = P_{k,n} U_n P_{k,n}$.

This yields

$$U_k \rho(G) U_k^\dagger = (P_{k,n} U_n P_{k,n}) \rho(G) (P_{k,n} U_n P_{k,n})^\dagger = P_{k,n} (U_n (P_{k,n} \rho(G) P_{k,n}^\dagger) U_n^\dagger) P_{k,n}^\dagger. \quad (10)$$

Therefore, the local unitary operation U_k on an n -qubit density matrix $\rho(G)$ defined by a graph G of order 2^n can be explained by the following switching procedure

$$G \mapsto^{p_{k,n}} G_{p_{k,n}} \mapsto^{U_n} G_{p_{k,n}}^{U_n} \mapsto^{p_{k,n}} G^{U_k} \quad (11)$$

where $U_n = I_2 \otimes \dots \otimes I_2 \dots \otimes U$ and $U \in \{X, Y, Z, H\}$. Then we have the following theorem.

Theorem 2 *Let G be a weighted undirected graph of order 2^n . Then $\rho(G^{U_k}) = U_k \rho(G) U_k^\dagger$ where $U_k = I_1 \otimes \dots \otimes I_2 \otimes U \otimes I_2 \otimes \dots \otimes I_2$, $k < n$ and $U \in \{X, Y, Z, H\}$ placed in the k -th position of the tensor product.*

Proof From (9), (10) and (11) we get the following equation:

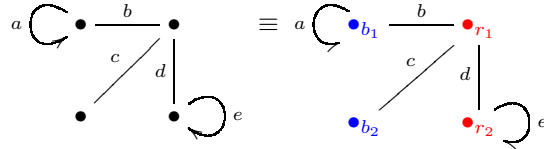
$$\begin{aligned} U_k \rho(G) U_k^\dagger &= U_k \frac{1}{\text{tr}(L(G))} L(G) U_k^\dagger \\ &= \frac{1}{\text{tr}(L(G))} U_k [D(G) + A(G)] U_k^\dagger \\ &= \frac{1}{\text{tr}(L(G))} P_{k,n} U_n P_{k,n} [D(G) + A(G)] (P_{k,n} U_n P_{k,n})^\dagger \\ &= \frac{1}{\text{tr}(L(G))} [D(G^{U_k}) + A(G^{U_k})]. \end{aligned}$$

$P_{k,n} U_n$ is a unitary matrix. Thus $\text{tr}(L(G)) = \text{tr}(L(G^k))$. Replacing it in the above equation we get,

$$U_k \rho(G) U_k^\dagger = \frac{1}{\text{tr}(L(G^k))} [D(G^{U_k}) + A(G^{U_k})] = \frac{1}{\text{tr}(L(G^k))} L(G^k) = \rho(G^{U_k}).$$

Hence proved.

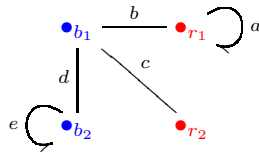
At the end of this section we would like to propose a simplified version of the graph theoretic interpretation of the operations X_n, Y_n and Z_n , discussed above. First, partition $V(G) = B \sqcup R$ into halves with colored vertices, say blue and red vertices, where the blue colored vertices are in $B = \{b_1, b_2, \dots, b_{2^{n-1}}\}$ and the red colored vertices are in $R = \{r_1, r_2, \dots, r_{2^{n-1}}\}$. Define two vertices of different colors say b_i and r_j as conjugate to each other if $i = j$. A loop (b_i, b_i) or (r_i, r_i) is an edge joining vertices of same color, that is, b_i and b_i or r_i and r_i . To illustrate all the transformations discussed above, we consider an example of a graph G of order 4, giving a 2-qubit state with edge weights a, b, c, d and e , as shown in the figure below.



Following changes in $E(G)$ switch G into G^{X_n} :

1. Given an edge joining vertices of same color (suppose r_i and r_j) in G , $E(G^{X_n})$ has a member joining corresponding conjugate vertices (b_i and b_j) with same edge weight.
2. Given an edge joining vertices of different colors (say (b_i, r_j) in G), $E(G^{X_n})$ has a member joining corresponding conjugate vertices (b_j, r_i) with same edge weight.

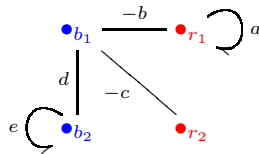
No change is required for edges (b_i, r_i) . For the particular example of the graph shown above, G^{X_n} is



Switching G to G^{Y_n} is equivalent to switching G to G^{X_n} with an additional operation:

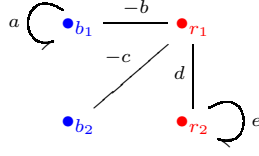
1. If there is an edge joining vertices of different colors in G , the new edge weight is equal to -1 times the old edge weight.

Thus, G^{Y_n} is



Switching G to G^{Z_n} is simplest as it does not change the location of any edge except the edge weight joining vertices of different colors. The new weight

is -1 times the old edge weight. Hence, G^{Z_n} for the graph G , introduced above, is



It is easy to check that $\rho(G^{U_n}) = U_n \rho(G) U_n^\dagger$ for $U = X, Y$ and Z in the above example.

4 CNOT gate and Bell state generation

CNOT gates occupy a central position in various quantum information processing tasks. They along with the Hadamard gate can be used for generating the two qubit maximally entangled Bell states from separable states. Here we adapt the switching techniques developed above to the *CNOT* gate, thereby providing a graphical method of Bell states generation.

Consider super-modules on $V(G)$ as a partition $\{\mathcal{C}_i : i = 0, 1, \dots, 2^{n-2} - 1\}$, where

$$\mathcal{C}_i = C_{2i} \cup C_{2i+1} = \{4i, 4i+1\} \cup \{4i+2, 4i+3\} = \{4i, 4i+1, 4i+2, 4i+3\}.$$

From a graph G with $|V(G)| = 2^n$, $n \geq 2$ we construct a graph $G^{C_{NOT}}(V(G^{C_{NOT}}), E(G^{C_{NOT}}))$, s.t. $\rho(G^{C_{NOT}}) = C_{NOT_n} \rho(G) C_{NOT_n}$, where, $C_{NOT_n} = I \otimes I \otimes \dots \otimes C_{NOT}$. Clearly $V(G^{C_{NOT}}) = V(G)$.

Procedure 2 Construct $E(G^{C_{NOT}})$ from $E(G)$ by graph switching

1. Changes inside a supermodule $\mathcal{C}_i : i = 0, 1, \dots, (2^{n-2} - 1)$ shall be as follows.
 - (a) No changes in the loops and edges inside module C_{2i}

$$\begin{aligned} (4i, 4i) \in E(G) &\Rightarrow (4i, 4i) \in E(G^{C_{NOT}}) \\ &w(4i, 4i)|_{G^{C_{NOT}}} = w(4i, 4i)|_G, \\ (4i+1, 4i+1) \in E(G) &\Rightarrow (4i+1, 4i+1) \in E(G^{C_{NOT}}) \\ &w(4i+1, 4i+1)|_{G^{C_{NOT}}} = w(4i+1, 4i+1)|_G, \\ (4i, 4i+1) \in E(G) &\Rightarrow (4i, 4i+1) \in E(G^{C_{NOT}}) \\ &w(4i, 4i+1)|_{G^{C_{NOT}}} = w(4i, 4i+1)|_G. \end{aligned} \tag{12}$$

(b) Do the following changes for the edges inside module C_{2i+1} .

$$\begin{aligned}
(4i+2, 4i+2) \in E(G) &\Rightarrow (4i+3, 4i+3) \in E(G^{C_{NOT}}), (4i+2, 4i+2) \notin E(G^{C_{NOT}}) \\
&\quad w(4i+3, 4i+3)|_{G^{C_{NOT}}} = w(4i+2, 4i+2)|_G, \\
(4i+3, 4i+3) \in E(G) &\Rightarrow (4i+2, 4i+2) \in E(G^{C_{NOT}}), (4i+3, 4i+3) \notin E(G^{C_{NOT}}) \\
&\quad w(4i+2, 4i+2)|_{G^{C_{NOT}}} = w(4i+3, 4i+3)|_G, \\
(4i+2, 4i+3) \in E(G) &\Rightarrow (4i+2, 4i+3) \in E(G^{C_{NOT}}) \\
&\quad w(4i+2, 4i+3)|_{G^{C_{NOT}}} = w(4i+2, 4i+3)|_G.
\end{aligned} \tag{13}$$

(c) Change the edges joining modules C_{2i} and C_{2i+1} of supermodule C_i .

$$\begin{aligned}
(4i, 4i+2) \in E(G) &\Rightarrow (4i, 4i+3) \in E(G^{C_{NOT}}), (4i, 4i+2) \notin E(G^{C_{NOT}}) \\
&\quad w(4i, 4i+3)|_{G^{C_{NOT}}} = w(4i, 4i+2)|_G, \\
(4i, 4i+3) \in E(G) &\Rightarrow (4i, 4i+2) \in E(G^{C_{NOT}}), (4i, 4i+3) \notin E(G^{C_{NOT}}) \\
&\quad w(4i, 4i+2)|_{G^{C_{NOT}}} = w(4i, 4i+3)|_G, \\
(4i+1, 4i+2) \in E(G) &\Rightarrow (4i+1, 4i+3) \in E(G^{C_{NOT}}), (4i+1, 4i+2) \notin E(G^{C_{NOT}}) \\
&\quad w(4i+1, 4i+3)|_{G^{C_{NOT}}} = w(4i+1, 4i+2)|_G, \\
(4i+1, 4i+3) \in E(G) &\Rightarrow (4i+1, 4i+2) \in E(G^{C_{NOT}}), (4i+1, 4i+3) \notin E(G^{C_{NOT}}) \\
&\quad w(4i+1, 4i+2)|_{G^{C_{NOT}}} = w(4i+1, 4i+3)|_G.
\end{aligned} \tag{14}$$

2. Changes in the edges joining different supermodules C_i and C_j for $i, j = 0, 1, \dots, (2^{n-2} - 1); i \neq j$ shall be as follows.

(a) No changes in the edges joining $C_{2i} \subset C_i$ and $C_{2j} \subset C_j$.

$$\begin{aligned}
(4i, 4j) \in E(G) &\Rightarrow (4i, 4j) \in E(G^{C_{NOT}}) \\
&\quad w(4i, 4j)|_{G^{C_{NOT}}} = w(4i, 4j)|_G, \\
(4i+1, 4j+1) \in E(G) &\Rightarrow (4i+1, 4j+1) \in E(G^{C_{NOT}}) \\
&\quad w(4i+1, 4j+1)|_{G^{C_{NOT}}} = w(4i+1, 4j+1)|_G, \\
(4i, 4j+1) \in E(G) &\Rightarrow (4i, 4j+1) \in E(G^{C_{NOT}}) \\
&\quad w(4i, 4j+1)|_{G^{C_{NOT}}} = w(4i, 4j+1)|_G, \\
(4i+1, 4j) \in E(G) &\Rightarrow (4i+1, 4j) \in E(G^{C_{NOT}}) \\
&\quad w(4i+1, 4j)|_{G^{C_{NOT}}} = w(4i+1, 4j)|_G.
\end{aligned} \tag{15}$$

(b) Change the edges joining $C_{2i} \subset \mathcal{C}_i$ and $C_{2j+1} \subset \mathcal{C}_j$ according to:

$$\begin{aligned}
(4i, 4j+2) \in E(G) &\Rightarrow (4i, 4j+3) \in E(G^{C_{NOT}}), (4i, 4j+2) \notin E(G^{C_{NOT}}) \\
&w(4i, 4j+3)|_{G^{C_{NOT}}} = w(4i, 4j+2)|_G, \\
(4i, 4j+3) \in E(G) &\Rightarrow (4i, 4j+2) \in E(G^{C_{NOT}}), (4i, 4j+3) \notin E(G^{C_{NOT}}) \\
&w(4i, 4j+2)|_{G^{C_{NOT}}} = w(4i, 4j+3)|_G, \\
(4i+1, 4j+2) \in E(G) &\Rightarrow (4i+1, 4j+3) \in E(G^{C_{NOT}}), (4i+1, 4j+2) \notin E(G^{C_{NOT}}) \\
&w(4i+1, 4j+3)|_{G^{C_{NOT}}} = w(4i+1, 4j+2)|_G, \\
(4i+1, 4j+3) \in E(G) &\Rightarrow (4i+1, 4j+2) \in E(G^{C_{NOT}}), (4i+1, 4j+3) \notin E(G^{C_{NOT}}) \\
&w(4i+1, 4j+2)|_{G^{C_{NOT}}} = w(4i+1, 4j+3)|_G.
\end{aligned} \tag{16}$$

(c) For the edges joining $C_{2i+1} \subset \mathcal{C}_i$ and $C_{2j} \subset \mathcal{C}_j$, the following changes need to be made:

$$\begin{aligned}
(4i+2, 4j) \in E(G) &\Rightarrow (4i+3, 4j) \in E(G^{C_{NOT}}), (4i+2, 4j) \notin E(G^{C_{NOT}}) \\
&w(4i+3, 4j)|_{G^{C_{NOT}}} = w(4i+2, 4j)|_G, \\
(4i+3, 4j) \in E(G) &\Rightarrow (4i+2, 4j) \in E(G^{C_{NOT}}), (4i+3, 4j) \notin E(G^{C_{NOT}}) \\
&w(4i+2, 4j)|_{G^{C_{NOT}}} = w(4i+3, 4j)|_G, \\
(4i+2, 4j+1) \in E(G) &\Rightarrow (4i+3, 4j+1) \in E(G^{C_{NOT}}), (4i+2, 4j+1) \notin E(G^{C_{NOT}}) \\
&w(4i+3, 4j+1)|_{G^{C_{NOT}}} = w(4i+2, 4j+1)|_G, \\
(4i+3, 4j+1) \in E(G) &\Rightarrow (4i+2, 4j+1) \in E(G^{C_{NOT}}), (4i+3, 4j+1) \notin E(G^{C_{NOT}}) \\
&w(4i+2, 4j+1)|_{G^{C_{NOT}}} = w(4i+3, 4j+1)|_G.
\end{aligned} \tag{17}$$

(d) Change the edges joining modules $C_{2i+1} \in \mathcal{C}_i$ and $C_{2j+1} \in \mathcal{C}_j$.

$$\begin{aligned}
(4i+2, 4j+4) \in E(G) &\Rightarrow (4i+3, 4j+3) \in E(G^{C_{NOT}}), (4i+2, 4j+4) \notin E(G^{C_{NOT}}) \\
&w(4i+3, 4j+3)|_{G^{C_{NOT}}} = w(4i+2, 4j+4)|_G, \\
(4i+3, 4j+3) \in E(G) &\Rightarrow (4i+2, 4j+2) \in E(G^{C_{NOT}}), (4i+3, 4j+3) \notin E(G^{C_{NOT}}) \\
&w(4i+2, 4j+2)|_{G^{C_{NOT}}} = w(4i+3, 4j+3)|_G, \\
(4i+2, 4j+3) \in E(G) &\Rightarrow (4i+2, 4j+3) \in E(G^{C_{NOT}}) \\
&w(4i+2, 4j+3)|_{G^{C_{NOT}}} = w(4i+2, 4j+3)|_G, \\
(4i+3, 4j+2) \in E(G) &\Rightarrow (4i+3, 4j+2) \in E(G^{C_{NOT}}) \\
&w(4i+3, 4j+2)|_{G^{C_{NOT}}} = w(4i+3, 4j+2)|_G.
\end{aligned} \tag{18}$$

Theorem 3 $\rho(G^{C_{NOT}}) = C_{NOTn}\rho(G)C_{NOTn}$.

Proof Proof follows from these block matrix multiplications.

$$C_{NOT_n} = I \otimes I \otimes \cdots \otimes C_{NOT} = \text{diag}\{I, X, I, X \dots I, X\}$$

$$C_{NOT_n} A(G) C_{NOT_n} = \begin{bmatrix} IC_0I & IC_{0,1}X & IC_{0,2}I & IC_{0,3}X & \dots \\ XC_{1,0}I & XC_1X & XC_{1,2}I & XC_{1,3}X & \dots \\ IC_{2,0}I & IC_{2,1}X & IC_2I & IC_{2,3}X & \dots \\ XC_{3,0}I & XC_{3,1}X & XC_{3,2}I & XC_3X & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

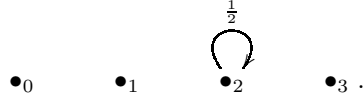
$$= \begin{bmatrix} C_{NOT}C_0C_{NOT} & C_{NOT}C_{0,1}C_{NOT} & \dots \\ C_{NOT}C_{1,0}C_{NOT} & C_{NOT}C_1C_{NOT} & \dots \\ \vdots & \vdots & \dots \end{bmatrix}$$

We now use graph switching techniques to depict the action of Hadamard and CNOT gates to generate Bell states from two qubit separable states. The structure of Bell states was shown earlier in [1].

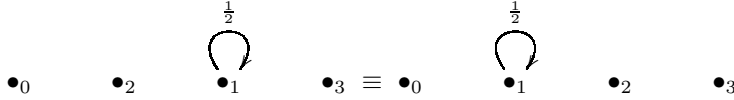
We begin with initial state $|10\rangle$. We operate a Hadamard gate on the first qubit followed by a CNOT gate to generate Bell state as follows,

$$|10\rangle \xrightarrow{H_1} \frac{1}{\sqrt{2}}(|00\rangle - |10\rangle) \xrightarrow{CNOT} \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle).$$

Graph, corresponding to state $|10\rangle$ $\langle 10|$, with vertex decomposition $\mathcal{C} = C_0 \cup C_1 = \{0, 1\} \cup \{2, 3\}$, is



To apply Hadamard gate on first qubit, i.e., H_1 , we first swap vertices. The graph changes to



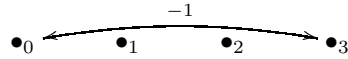
Apply H_2 and get a new graph



To finish H_1 we swap it again. Graph after completing Hadamard operation is



Now apply CNOT operation. Following the procedure applied above, the new graph represents the state $\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$ [1].



Similarly all other Bell states can be generated graph theoretically.

5 Conclusion

In this work we establish a proof of principle for representing quantum states and local unitaries graph theoretically. In particular, quantum states are described by the signless Laplacian matrix of their graph representation. We work out in detail the graph switching operations that correspond to some important local unitaries on n qubits.

While this has obvious significance in quantum information processing, we think that this may have impact on foundational issues as well. Essentially, by representing quantum superposition as a weighted edge, (to give a dramatic slant) our approach geometrizes non-realism, and herein lies its appeal. The full scope of this approach and its generalization to the hypergraph formalism [21] will be discussed in future works.

This work is, hopefully, a stepping stone towards a graph theoretical understanding of issues in quantum foundations and quantum information.

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