3

Graph Theoretic Aspects of Quantum Dynamics

Dynamics is concerned with a study of motion of elements. In general we study changes in motion, stability, and state of an element with time by a system of differential equations depending on time. Quantum dynamics is the quantum version of classical dynamics. Unitary evolution of quantum state is a crucial component of quantum dynamics. A number of unitary operators act as quantum gates which are quantum mechanical counterparts of classical logic gates. In this chapter, we present a graph theoretical analog of these logic gate operations. The bulk of the work presented in this chapter follows [Dutta et al., 2016a].

3.1 AN INTRODUCTION TO UNITARY EVOLUTION AND GRAPH SWITCHING

We have seen in Chapter 2 that in quantum mechanics a state is represented by a state vector belonging to an appropriate Hilbert space or a density matrix of appropriate order. Time evolution of the quantum state is given by the time dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(\mathbf{r},t)\right\rangle = \hat{H}\left|\Psi(\mathbf{r},t)\right\rangle, \tag{3.1}$$

where $|\Psi(\mathbf{r},t)\rangle$ is state of the particle at time t and position **r**, and $\hat{H}$ is the system Hamiltonian, a Hermitian matrix. Assuming a time independent Hamiltonian H, a solution of the equation may be given by,

$$|\Psi'\rangle = \exp\left(-\frac{i}{\hbar}\hat{H}t\right)|\Psi\rangle, \tag{3.2}$$

As $\hat{H}$ is a Hermitian matrix, $\exp(-\frac{i}{\hbar}\hat{H}t)$ is a unitary operator. Thus, evolution of quantum states are given by unitary operations on them. Given any unitary operator U, $UU^\dagger = U^\dagger U = I$ where $U^\dagger$ is the conjugate transpose of U. If $|\Psi'\rangle$ be the new state after a unitary evolution U on the state $|\Psi\rangle$, then $|\Psi'\rangle$ can be represented by,

$$|\Psi'\rangle = U|\Psi\rangle. \tag{3.3}$$

If the quantum system is represented by an ensemble of quantum states $\{p_i, |\psi_i\rangle\}$ the unitary evolution on the system is given by $\{p_i, U|\psi_i\rangle\}$. Recall that, in terms of density matrix the system can be given by $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. If ρ' be the new density matrix after the unitary evolution then,

$$\rho' = \sum_i p_i U|\psi_i\rangle\langle\psi_i| U^\dagger = U\left(\sum_i p_i|\psi_i\rangle\langle\psi_i|\right)U^\dagger = U\rho U^\dagger. \tag{3.4}$$

Definition 3.1. Local and global unitary operator: *Consider the state* $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes |\psi_n\rangle$ *such that* $|\psi\rangle \in \mathcal{H}_i$. *Let* U *be an unitary operator acting on* $|\psi\rangle$. *If we can represent* $U = U_1 \otimes U_2 \otimes \cdots \otimes U_n$ *where* U_i *acts on the state vectors belonging to* $\mathcal{H}_i$, *then* U *is called a local unitary operator. Otherwise* U *is a global unitary operator.*

Example 3.1. *Consider the unitary operator of order* 4

$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{3.5}$$

Note that, we can not write $CNOT = U_1 \otimes U_2$ *such that* U_1*, and* U_2 *act on states in* $\mathcal{H}^{(2)}$*. Thus,* $CNOT$ *is a global unitary operator. But, for another unitary operator*

$$U = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{3.6}$$

Therefore, U *is a local unitary operator.*

Unitary operators of order 2 forms an algebraic group under matrix multiplication, which is denoted by $U(2)$. The special unitary group is denoted by $SU(2)$ which contains all unitary matrices of order 2 and determinant 1. Formally we can write,

$$SU(2) = \left\{ \begin{bmatrix} \alpha & -\overline{\beta} \\ \beta & \overline{\alpha} \end{bmatrix} : \alpha, \beta \in \mathbb{C}, |\alpha|^2 + |\beta|^2 = 1 \right\} = \left\{ \begin{bmatrix} e^{i\phi_1}\cos\theta & e^{i\phi_2}\sin\theta \\ -e^{-i\phi_2}\sin\theta & e^{-i\phi_1}\cos\theta \end{bmatrix} : |e^{i\phi_1}| = |e^{i\phi_2}| = 1 \right\}. \tag{3.7}$$

There is a Lie algebra corresponding to $SU(2)$ which is given by,

$$su(2) = \left\{ \begin{bmatrix} ia & -\overline{z} \\ z & -ia \end{bmatrix} : a \in \mathbb{R}, z \in \mathbb{C} \right\}, \tag{3.8}$$

and is generated by the Pauli matrices $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, and $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$.

In quantum computation, we use the Pauli X, Y, Z, and the Hadamard $H = \frac{X+Z}{\sqrt{2}}$ operators as quantum gates. They are quantum mechanical counterparts of logic gates, which play a key role in classical computation. We use Kronecker products of their combinations on the system of qubits, which forms a quantum circuit. Therefore, a unitary evolution of a multi-qubit quantum system can be performed by local unitary operators of the form

$$U_k = U^{(1)} \otimes \cdots \otimes U^{(k-1)} \otimes U \otimes U^{(k+1)} \otimes \cdots \otimes U^{(n)}, \tag{3.9}$$

where $U \in \{X, Y, Z, H\}$ and $U^{(j)} = I_2$ the identity matrix of order 2 when $j \neq k$, and $k = 1, 2, \dots, n$. Here U_k acts on the k-th qubit in an n-qubit system. Now we transit to the graph theory for further development.

We have shown that there is a quantum state represented by the density matrix $\rho(G)$ corresponding to a graph G. Recall, from the subsection 2.3.1, that a single qubit can be represented by a graph with two vertices (see figure 2.4). In general, a n-qubit quantum state is represented by a graph with 2^n vertices partitioned into 2^{n-1} clusters. Thus, a unitary evolution on n-qubit quantum state can be identified as a combinatorial operation on a graph with 2^n vertices. In graph theory, such types of operations are called graph switching. Two graphs $G = (V(G), E(G))$ and $H = (V(H), E(H))$ are switching equivalent if $V(H) = V(G)$, and $E(H)$ is given by $E(G)$ after removing/adding some weighted edges and/or altering weights of the edges in G. In this context, Seidel switching is a well known technique for generating co-spectral graphs.

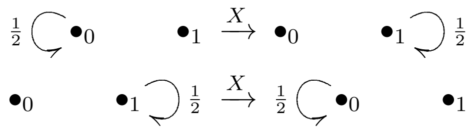


Figure 3.1 : X-gate operation on $|0\rangle$ and $|1\rangle$.

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 defined in equation (3.9). The unitary matrix U_k of order 2^n given in (3.9) is a local unitary transformation acting on the Hilbert space $\mathbb{C}^{2^n} \equiv \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2$. We show that when U_k is applied on a density matrix of a n-qubit quantum state $\rho(G)$, obtained by signless Laplacian matrix associated with a weighted graph G, the resulting unitary transformation can be realized by suitable graph switchings. We call G and G^{U_k} as local unitary equivalent graphs.

In this chapter, we like to visualize graph theoretic interpretation of a number of quantum gates widely used in quantum computation [Dutta et al., 2016a]. For simplicity, we restrict our attention to weighted undirected graphs and the density matrices corresponding to their signless Laplacian matrices. For Laplacian matrices all the constructions will be equivalent and hence is not discussed here.

3.2 OPERATIONS ON SINGLE QUBIT QUANTUM STATES

We begin with the density matrices of the simplest quantum state $|0\rangle$ and$|1\rangle$, that is $\rho_0 = |0\rangle\langle 0|$ and $\rho_1 = |1\rangle\langle 1|$, which corresponds to the graphs depicted in 2.4. Useful unitary operations on qubits are generated by the Pauli X, Y, Z and the Hadamard H transformation. We now represent these evolutions as graphical operations:

1. X **gate:** The X gate is considered as a quantum equivalent to the NOT gate in classical computation which changes the bits 0 to 1 and 1 to 0. As, $X|0\rangle = |1\rangle$ and $X|1\rangle = |0\rangle$ in terms of density matrices, $X\rho_0 X^{\dagger} = \rho_1$ and $X\rho_1 X^{\dagger} = \rho_0$. 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. The graphical changes are similar for ρ_1, which are illustrated in the figure 3.1.

2. Y **gate:** The Y gate acts as X gate with an additional phase shift. Precisely, $Y|0\rangle = i|1\rangle$ and $Y|1\rangle = -i|0\rangle$. Clearly, $Y\rho_0 Y^{\dagger} = \rho_1$ and $Y\rho_1 Y^{\dagger} = \rho_0$. The graphical representation of Y gate is equivalent to that of X above.

3. Z **gate:** The Z gate keeps $|0\rangle$ unchanged and converts $|1\rangle$ to $-|1\rangle$. Therefore, $Z|0\rangle = |1\rangle$ and $Z|1\rangle = -|1\rangle$. Here $Z\rho_0 Z^{\dagger} = \rho_0$ and $Z\rho_1 Z^{\dagger} = \rho_1$. Thus their is no change in the graph.

4. H **gate:** We have $H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. Note that, $H\rho_0 H^{\dagger} = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$. It is the signless Laplacian density matrix corresponding to a graph with two vertices and an edge. Similarly, $H\rho_1 H^{\dagger} = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$. It corresponds to a graph with two vertices with an edge of weight -1. The graphical representations of H are depicted in the figure 3.2.

Although the graphical changes for Y and Z gate are insignificant for a single qubit, we may find differences when multi-qubit systems are considered, as in the next section.

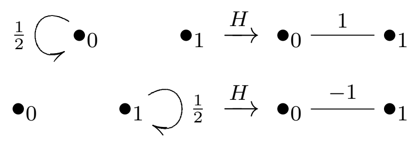


Figure 3.2 : H-gate operation on $|0\rangle$ and $|1\rangle$.

3.3 OPERATIONS ON MULTI-QUBIT QUANTUM STATES

Recall the unitary operator U_k acting on the n qubit quantum state mentioned in the equation (3.9). For simplicity we start our calculations with U_n which is,

$$U_n = U^{(1)} \otimes U^{(2)} \cdots \otimes U^{(n-1)} \otimes U, \tag{3.10}$$

where $U^{(i)} = I$, the identity matrix of order 2, for $i = 1, 2, \dots (n-1)$ and $U \in \{X, Y, Z, H\}$. Therefore, the quantum gate U acts on n-th qubit in an n-qubit quantum state and the other qubits remain unaltered. Later we shall establish an isomorphism to calculate U_k in terms of U_n. The operator U_n is beneficial for simplifying our calculations as it has a structure of diagonal block matrix as follows,

$$U_n = \text{diag}\{U, U, \dots U\}, \tag{3.11}$$

that is, its 2×2 diagonal blocks are the unitary matrix U.

In subsection 2.2.6, we have seen that an n qubit system can be represented by a graph with 2^{n-1} clusters each containing two vertices. That is,

$$V(G) = C_1 \cup C_2 \cup \cdots \cup C_{2^{n-1}} \text{ such that } C_\mu = \{v_{\mu,1}, v_{\mu,2}\}. \tag{3.12}$$

Recall that the subgraph $\langle C_\mu \rangle$ is the induced subgraph generated by C_μ. Its adjacency matrix is given by the diagonal block $A_{\mu,\mu}$. The subgraph $\langle C_\mu, C_\nu \rangle$ consists of vertex set $C_\mu \cup C_\nu$ and edges joining vertices belonging to different clusters. Its adjacency matrix is given by,

$$A(\langle C_\mu, C_\nu \rangle) = \begin{bmatrix} 0 & A_{\mu,\nu} \\ A_{\nu,\nu} & 0 \end{bmatrix}. \tag{3.13}$$

The clustering partition the density matrix $\rho(G)$ into blocks. Therefore,

$$\rho(G) = \begin{bmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{12^{n-1}} \\ \rho_{21} & \rho_{22} & \cdots & \rho_{22^{n-1}} \\ \cdots & \cdots & \cdots & \cdots \\ \rho_{2^{n-1}1} & \rho_{2^{n-1}2} & \cdots & \rho_{2^{n-1}2^{n-1}} \end{bmatrix}. \tag{3.14}$$

As U_n is a block diagonal matrix,

$$\rho(G^{U_n}) = U_n \rho(G) U_n^\dagger = \begin{bmatrix} U\rho_{11}U^\dagger & U\rho_{12}U^\dagger & \cdots & U\rho_{12^{n-1}}U^\dagger \\ U\rho_{21}U^\dagger & U\rho_{22}U^\dagger & \cdots & U\rho_{22^{n-1}}U^\dagger \\ \cdots & \cdots & \cdots & \cdots \\ U\rho_{2^{n-1}1}U^\dagger & U\rho_{2^{n-1}2}U^\dagger & \cdots & U\rho_{2^{n-1}2^{n-1}}U^\dagger \end{bmatrix}. \tag{3.15}$$

Clearly, $V(G^{U_n}) = V(G)$ and $E(G^{U_n})$ can be expressed in terms of some well defined changes in $E(G)$ depending on U.

For a simplified description, we colour the vertices $v_{\mu,1}$ with blue and $v_{\mu,2}$ with red for all $\mu = 1, 2, \dots 2^{n-1}$. Therefore, $V(G) = B \cup R$ where $B = \{v_{\mu,1} : \mu = 1, 2, \dots 2^{n-1}\}$, and $R = \{v_{\mu,2} :$

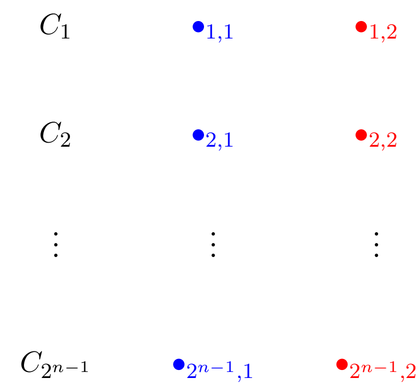


Figure 3.3 : Colouring on vertices in clusters for graphs representing multi-qubit systems

$\mu = 1, 2, \dots 2^{n-1}\}$. The coloured grid structure is shown in the figure 3.3. We call two vertices $v_{\mu,1}$ and $v_{\mu,2}$ conjugate to each other. Also we consider a loop $(v_{\mu,i}, v_{\mu,i})$ as an edge joining vertices of same colour Now, we are in a position to describe switching procedures which are graph theoretic analogues of different quantum gate operations.

3.3.1 X Gate

We consider the local unitary operation $X_n = I \otimes I \otimes I \otimes \cdots \otimes X$. In an n-qubit system, it is equivalent of X gate operation on the n-th qubit keeping other qubits unchanged. Let G^{X_n} be the graph derived from G such that $\rho(G^{X_n}) = X_n \rho(G) X_n^\dagger$. Here we enlist the switching procedure to convert G to G^{X_n}. We consider the procedure as the graph theoretical analogue of X gate operation on n-th qubit.

Procedure 3.1. Construct $E(G^{X_n})$ from $E(G)$: *Following changes in $E(G)$ switch G into G^{X_n}:*

1. *Given an edge joining vertices of same colour in G, $E(G^{X_n})$ has a member joining corresponding conjugate vertices with same edge weight.*
2. *Given an edge joining vertices of different colours in G, $E(G^{X_n})$ has a member joining corresponding conjugate vertices with same edge weight.*

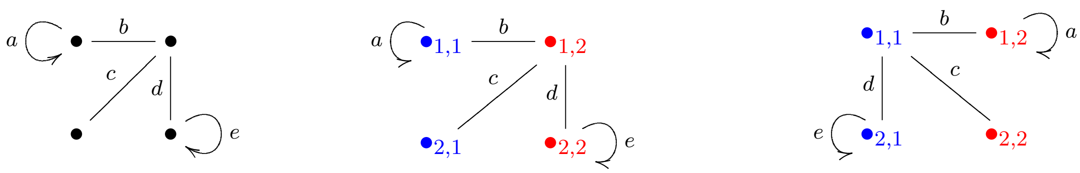
No change is required for other edges.

Example 3.2. *Consider a graph G of order 4 with edge weights a, b, c, d and e, depicted in the figure 3.4a. Note that, $\rho(G)$ a 2-qubit state. After coloring the vertices we get the figure depicted in 3.4b. In the figure 3.4c, we depict the graph G^{X_2}. Density matrices of these graphs are*

$$\rho(G) = \frac{1}{d}\begin{bmatrix} 2a+b & b & 0 & 0 \\ b & b+c+d & c & d \\ 0 & c & c & 0 \\ 0 & d & 0 & d+2e \end{bmatrix} \text{ and } \rho(G^{X_2}) = \frac{1}{d}\begin{bmatrix} b+c+d & b & d & c \\ b & 2a+b & 0 & 0 \\ d & 0 & d+2e & 0 \\ c & 0 & 0 & c \end{bmatrix}. \tag{3.16}$$

where $d = 2a + 4b + 4c + 4d + 2e$. Now we can see $\rho(G^{X_2}) = X_2 \rho(G) X_2^\dagger$.

Theorem 3.1. *Let G^{X_n} be the graph obtained from graph G using the procedure 3.1, then $\rho(G^{X_n}) = X_n \rho(G) X_n^\dagger$.*



(a) The graph G

(b) The graph G after coloring.

(c) The graph G^{X_2} after switching.

Figure 3.4 : Graph switching operation equivalent to X gate.

Proof. The adjacency matrix of induced subgraph $\langle C\mu \rangle$ is given by $A_{\mu,\mu}$. Note that,

$$\begin{aligned} A_{\mu,\mu} &= \begin{bmatrix} w(v_{\mu,1}, v_{\mu,1}) & w(v_{\mu,1}, v_{\mu,2}) \\ w(v_{\mu,1}, v_{\mu,2}) & w(v_{\mu,2}, v_{\mu,2}) \end{bmatrix} \Rightarrow XA_{\mu,\mu}X^{\dagger} = \begin{bmatrix} w(v_{\mu,2}, v_{\mu,2}) & w(v_{\mu,1}, v_{\mu,2}) \\ w(v_{\mu,1}, v_{\mu,2}) & w(v_{\mu,1}, v_{\mu,1}) \end{bmatrix}, \\ \text{and } A_{\mu,\nu} &= \begin{bmatrix} w(v_{\mu,1}, v_{\nu,1}) & w(v_{\mu,1}, v_{\nu,2}) \\ w(v_{\mu,1}, v_{\nu,2}) & w(v_{\mu,2}, v_{\nu,2}) \end{bmatrix} \Rightarrow XA_{\mu,\nu}X^{\dagger} = \begin{bmatrix} w(v_{\mu,2}, v_{\nu,2}) & w(v_{\mu,1}, v_{\nu,2}) \\ w(v_{\mu,1}, v_{\nu,2}) & w(v_{\mu,1}, v_{\nu,1}) \end{bmatrix}. \end{aligned} \tag{3.17}$$

Therefore the edges obtained by joining vertices of same colour is replaced by the edges joining the conjugate vertices. Also note that the edge weight inside the module C_i remains unchanged. They reflect procedure 3.1. Combining the changes in the block matrices we get, $A(G^{X_n}) = X_n A(G) X_n^{\dagger}$. Also note that, $d(v_{\mu,1})|_{G^{X_n}} = d(v_{\mu,2})|_G$ and $d(v_{\mu,2})|_{G^{X_n}} = d(v_{\mu,2})|_G$. Hence,

$$\begin{aligned} D(G^n) &= \text{diag}\{D_i^{(X_n)} : i = 0, 1, \dots\} = X_n D(G) X_n^{\dagger} \\ Q(G^{X_n}) &= D(G^{X_n}) + A(G^{X_n}) = X_n (D(G) + A(G)) X_n^{\dagger} \end{aligned} \tag{3.18}$$

Also, $\text{trace}(Q(G^{X_n})) = \text{trace}(Q(G))$. Therefore, $\rho(G^{X_n}) = X_n \rho(G^{X_n}) X_n^{\dagger}$. Hence the proof. □

3.3.2 Y gate

Here, we consider the local unitary operation $Y_n = I \otimes I \otimes I \otimes \cdots \otimes Y$, which is equivalent to the Y gate operation on n-th qubit in an n qubit system. Let G^{Y_n} be the graph generated from G after suitable changes in $E(G)$ such that $\rho(G^{Y_n}) = Y_n \rho(G) Y_n^{\dagger}$. The changes in edge set are described in the following procedure.

Procedure 3.2. Construct $E(G^{Y_n})$ from $E(G)$: *Following changes in $E(G)$ switch G into G^{Y_n}: Follow the procedure 3.1 with an additional operation mentioned below:*

1. *If there is an edge joining vertices of different colours in G, the new edge weight is equal to -1 times the old edge weight in the graph G^{Y_n}.*

Example 3.3. *Consider the graph G of order 4 with edge weights a, b, c, d and e, depicted in the figure 3.5. After switching operation, we get the new graph depicted in the figure 3.5b. Note that, we have considered the graph of the last example. Difference between the X and Y operations are brought out by the weights of edges joining two vertices of different color. After Y operation edge weights of these edges becomes negative. Consider the density matrix*

$$\rho(G^{Y_2}) = \frac{1}{d} \begin{bmatrix} b + c + d & -b & d & -c \\ -b & 2a + b & 0 & 0 \\ d & 0 & d + 2e & 0 \\ -c & 0 & 0 & c \end{bmatrix}. \tag{3.19}$$

We can check that $\rho(G^{Y_2}) = Y_2 \rho(G) Y_2^{\dagger}$.

(a) The graph G. **(b)** The graph G^{Y_2} after switching.

Figure 3.5 : Graph switching operation equivalent to Y gate.

Theorem 3.2. *Let G^{Y_n} be a graph obtained from G after the switching operation mentioned in the procedure 3.2. Then $\rho(G^{Y_n}) = Y_n \rho(G) Y_n^\dagger$.*

Proof. First consider the diagonal block matrices for $A(G)$ and $A(G^{Y_n})$.

$$A_{\mu,\mu} = \begin{bmatrix} w(v_{\mu,1}, v_{\mu,1}) & w(v_{\mu,1}, v_{\mu,2}) \\ w(v_{\mu,1}, v_{\mu,2}) & w(v_{\mu,2}, v_{\mu,2}) \end{bmatrix} \Rightarrow Y A_{\mu,\mu} Y^\dagger = \begin{bmatrix} w(v_{\mu,2}, v_{\mu,2}) & -w(v_{\mu,1}, v_{\mu,2}) \\ -w(v_{\mu,1}, v_{\mu,2}) & w(v_{\mu,1}, v_{\mu,1}) \end{bmatrix}. \quad (3.20)$$

Note that, the loops at $v_{\mu,1}$ and $v_{\mu,2}$ change their positions keeping edge weight unchanged. Also, the edge joining vertices of two different colours remains unchanged but the edge weight becomes negative.

Now consider changes in a non-diagonal block.

$$A_{\mu,\nu} = \begin{bmatrix} w(v_{\mu,1}, v_{\nu,1}) & w(v_{\mu,1}, v_{\nu,2}) \\ w(v_{\mu,1}, v_{\nu,2}) & w(v_{\mu,2}, v_{\nu,2}) \end{bmatrix} \Rightarrow Y A_{\mu,\nu} Y^\dagger = \begin{bmatrix} w(v_{\mu,2}, v_{\nu,2}) & -w(v_{\mu,1}, v_{\nu,2}) \\ -w(v_{\mu,1}, v_{\nu,2}) & w(v_{\mu,1}, v_{\nu,1}) \end{bmatrix}. \quad (3.21)$$

This reflects the fact that the edges between the vertices of same colours change their positions between conjugate vertices of the opposite colours Also, the edges joining vertices of different colours change their position by joining their conjugate vertices and the edge weights become negative.

Combining all the block matrices we get $A(G^{Y_n}) = Y_n A(G) Y_n^\dagger$. Also note that, $d(v_{\mu,1})_{G^{Y_n}} = d(v_{\mu,2})_G$ and $d(v_{\mu,2})_{G^{Y_n}} = d(v_{\mu,1})_G$. Hence,

$$\begin{aligned} D(G^n) &= \text{diag}\{D_i^{(Y_n)} : i = 0, 1, \dots\} = Y_n D(G) Y_n^\dagger \\ Q(G^{Y_n}) &= D(G^{Y_n}) + A(G^{Y_n}) = Y_n [D(G) + A(G)] Y_n^\dagger = Y_n Q(G) Y_n^\dagger \end{aligned} \quad (3.22)$$

Also, $\text{trace}(Q(G^{Y_n})) = \text{trace}(Q(G))$. Therefore, $\rho(G^{Y_n}) = Y_n \rho(G) Y_n^\dagger$. Hence the proof. □

3.3.3 Z gate

Consider the Z gate operation on the n-th qubit in an n qubit system. The local unitary operation involved here is $Z_n = I \otimes I \otimes I \otimes \cdots \otimes Z$. Let G^{Z_n} be the graph generated from G such that $\rho(G^{Z_n}) = Z \rho(G) Z^\dagger$.

Procedure 3.3. Construct $E(G^{Z_n})$ from $E(G)$: *Following changes in $E(G)$ switch G into G^{Z_n}:*

1. *Multiply (-1) with the edge weight of the edge joining two vertices of different colours*

Example 3.4. *We consider the graph G depicted in the figure 3.6. Note that the graph structure remains unchanged after Z_2 operation. Only the edges joining two vertices of different colour have negative weight.*

(a) The graph G.

(b) The graph G^{Z_2} after switching.

Figure 3.6 : Graph switching operation equivalent to Z gate operation.

The density matrix of G^{Z_2} is given by

$$\rho(G^{Z_2}) = \begin{bmatrix} 2a+b & -b & 0 & 0 \\ -b & b+c+d & -c & d \\ 0 & -c & c & 0 \\ 0 & d & 0 & d+2e \end{bmatrix} = Z_2 \rho(G) Z_2^{\dagger}. \tag{3.23}$$

Theorem 3.3. *Let G^{Z_n} be a graph generated by the procedure 3.3 from the graph G. Then, $\rho(G^{Z_n}) = Z_n \rho(G) Z_n^{\dagger}$.*

Proof. Consider changes in the diagonal blocks of the adjacency matrices $A(G)$ and $A(G^{Z_n})$ under Z_n operation,

$$A_{\mu,\mu} = \begin{bmatrix} w(v_{\mu,1}, v_{\mu,1}) & w(v_{\mu,1}, v_{\mu,2}) \\ w(v_{\mu,1}, v_{\mu,2}) & w(v_{\mu,2}, v_{\mu,2}) \end{bmatrix} \Rightarrow Z A_{\mu,\mu} Z^{\dagger} = \begin{bmatrix} w(v_{\mu,1}, v_{\mu,1}) & -w(v_{\mu,1}, v_{\mu,2}) \\ -w(v_{\mu,1}, v_{\mu,2}) & w(v_{\mu,2}, v_{\mu,2}) \end{bmatrix}. \tag{3.24}$$

Hence, the loops at $v_{\mu,1}$ and $v_{\mu,2}$ remain unchanged. Also, the edge weight of the edge joining two vertices of different colours inside the cluster C_μ is multiplied by -1. Now consider changes in non-diagonal block,

$$A_{\mu,\nu} = \begin{bmatrix} w(v_{\mu,1}, v_{\nu,1}) & w(v_{\mu,1}, v_{\nu,2}) \\ w(v_{\mu,1}, v_{\nu,2}) & w(v_{\mu,2}, v_{\nu,2}) \end{bmatrix} \Rightarrow Z A_{\mu,\nu} Z^{\dagger} = \begin{bmatrix} w(v_{\mu,1}, v_{\nu,1}) & -w(v_{\mu,1}, v_{\nu,2}) \\ -w(v_{\mu,1}, v_{\nu,2}) & w(v_{\mu,2}, v_{\nu,2}) \end{bmatrix}. \tag{3.25}$$

It reflects that the edge weights of the edges joining vertices of different colours are multiplied by -1. There is no change in any other edges and their locations. It is important that there is no interchange between two constitutive rows. Thus, $d(v_{\mu,1})|_{G^{Z_n}} = d(v_{\mu,1})|_G$ and $d(v_{\mu,2})|_{G^{Z_n}} = d(v_{\mu,2})|_G$. Hence,

$$\begin{aligned} D(G^{Z_n}) &= \text{diag}\{Z.D_i.Z^{\dagger} : i = 0, 1, \dots\} = Z_n D(G) Z_n^{\dagger} = D(G) \\ Q(G^{Z_n}) &= D(G^{Z_n}) + A(G^{Z_n}) = Z_n [D(G) + A(G)] Z_n^{\dagger} = Z_n Q Z_n^{\dagger}. \end{aligned} \tag{3.26}$$

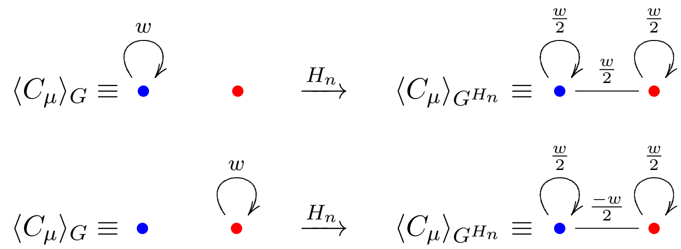
Also, trace$(Q(G^{Z_n}))$ = trace$(Q(G))$. Therefore, $\rho(G^{Z_n}) = Z_n \rho(G^{Z_n}) Z_n^{\dagger}$. Hence, the proof. □

3.3.4 H Gate

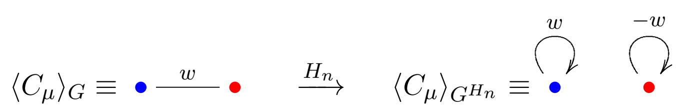
Next, we discuss the graph theoretical approach for applying Hadamard gate on a product state. Recall that, Hadamard gate is given by $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$. We construct a new graph $G^{H_n} = (V(G^{H_n}), E(G^{H_n}))$ from $G = (V(G), E(G))$ such that $\rho(G^{H_n}) = H_n \rho(G) H_n^{\dagger}$ where $H_n = I \otimes I \otimes \cdots \otimes I \otimes H$ which is equivalent to H gate operation on n-th qubit of an n-qubit quantum state. Clearly $V(G) = V(G^{H_n})$ and $E(G^{H_n})$ will be constructed from $E(G)$ using the following procedure.

Procedure 3.4. Construct $E(G^{H_n})$ from $E(G)$

1. *A loop on a blue colour vertex in G at the cluster C_μ will produce loops on both the vertices and an edge joining them at the cluster C_μ of the graph G^{H_n}. If w is the loop weight in G, weights of loops and edges in G^{H_n} will be $\frac{w}{2}$. A loop on a red vertex will generate loops on vertices, similarly. But the edge will have negative weight. Pictorially,*

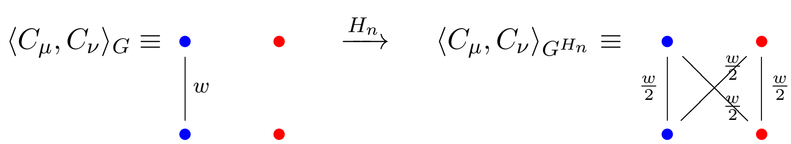


2. *An edge of weight w joining two vertices in a cluster C_μ of G will produce two loops on the vertices of C_μ in G^{H_n}. Loop weights will be w and $-w$ for blue and red colour vertices. Pictorially,*

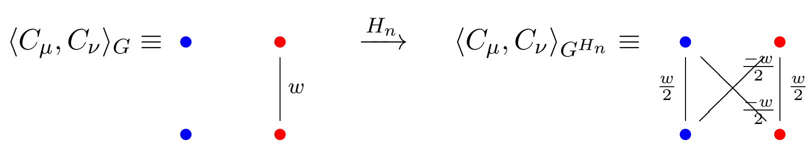


3. *An edge of weight w joining two vertices of in $\langle C_\mu, C_\nu \rangle$ of G will produce all the edges in $\langle C_\mu, C_\nu \rangle$ of G^{H_n}. Edge weights in $\langle C_\mu, C_\nu \rangle_{G^{H_n}}$ will be as follows:*

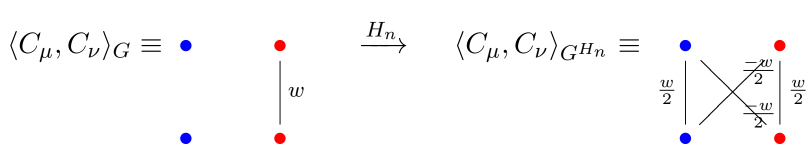
   a) *If the edge joins two blue vertices in G weights of all the edges in G^{H_n} will be $\frac{w}{2}$. Pictorially,*



   b) *If the edge joins two red vertices in G then weight of edge joining same color vertices will be $\frac{w}{2}$ and $\frac{-w}{2}$ for others. Pictorially,*



   c) *If the edge joins a blue and a red vertices in G then weight of edge joining same colour vertices will be $\frac{w}{2}$ and $\frac{-w}{2}$ for others. Pictorially,*



Theorem 3.4. *Let G^{H_n} be the graph generated from G using the above procedure, then $\rho(G^{H_n}) = H_n \rho(G) H_n^\dagger$.*

Proof. The adjacency submatrix corresponding to the subgraph $\langle C_\mu \rangle$ is given by $A_{\mu,\mu}$. Then the adjacency submatrix corresponding to $\langle C_\mu \rangle_{G^{H_n}}$ is given by $HA_{\mu,\mu}H^\dagger$. Now we observe the changes mentioned in the procedure by comparing two subgraphs $\langle C_\mu \rangle_G$ and $\langle C_\mu \rangle_{G^n}$. Similarly, we may find the changes between the subgraphs $\langle C_\mu, C_\nu \rangle_G$ and $\langle C_\mu, C_\nu \rangle_{G^n}$.

Also note that $d(v_{\mu,2})|_{G^{H_n}} = d(v_{\mu,1})|_G$ and $d(v_{\mu,1})|_{G^{H_n}} = d(v_{\mu,2})|_G$. Thus,

$$D(G^n) = \text{diag}\{D_i^{(H)} : i = 0, 1, \dots\} = H_n D(G) H_n^\dagger$$
$$Q(G^{H_n}) = D(G^{H_n}) + A(G^{H_n}) = H(D(G) + A(G))H^\dagger.$$

Combining we get, $\text{trace}(Q(G^{H_n})) = \text{trace}(Q(G))$ and $\rho(G^{H_n}) = H_n \rho(G^{H_n}) H_n^\dagger$. Hence the proof. □

3.3.5 Operation on arbitrary qubit

In the proceeding subsections we have studied the graph switching techniques corresponding to the local unitary operators X_n, Y_n, Z_n and H_n acting on a density matrix $\rho(G)$ representing an n-qubit quantum state defined by the signless Laplacian associated with a weighted undirected graph G. Now we focus on the local unitary operators U_k when $k < n$ mentioned in the equation (3.9). Therefore, $U_k = U^{(1)} \otimes \cdots \otimes U^{(k-1)} \otimes U \otimes U^{(k+1)} \otimes \cdots \otimes U^{(n)}$, where $U \in \{X, Y, Z, H\}$ and $U^{(j)} = I_2$ the identity matrix of order 2 when $j \neq k$, and $k < n$.

Recall that, the graph G represents a density matrix $\rho(G)$ corresponding to an n-qubit quantum state. Thus, number of vertices in G is 2^n. Therefore, we may write $V(G) = \{0,1\}^n \equiv \{0, 1, \dots, 2^n - 1\}$ such that a vertex $j \in V(G)$ is represented by a sequence of 0, and 1. The labelling of the vertices of G is determined by the lexicographic ordering defined on $\{0,1\}^n$. For example, if $n = 2$ the labelled vertex set is given by $V(G) = \{00, 01, 10, 11\}$. Now, we can consider a permutation $p_{k,n} : \{0,1\}^n \to \{0,1\}^n$ such that $p(x_1 x_2 \dots x_{k-1} x_k x_{k+1} \dots x_n) = x_1 x_2 \dots x_{k-1} x_n x_{k+1} \dots x_k$ where $x_i \in \{0,1\}$. Thus, given the standard lexicographic ordering on $\{0,1\}^n$, $p_{k,n}$ introduces a relabelling of the vertices. Let $P_{k,n}$ be the unique permutation matrix associated with $p_{k,n}$. Then it is easy to verify that

$$A(G_{p_{k,n}}) = P_{k,n} A(G) P_{k,n}^\dagger, \quad D(G_{p_{k,n}}) = P_{k,n} D(G) P_{k,n}^\dagger \tag{3.27}$$

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

$$U_k \rho(G) U_k^\dagger = (P_{k,n} U_n P_{k,n}) \rho(G) (P_{k,n} U_n P_{k,n})^\dagger = P_{k,n} (U_n (P_{k,n} \rho(G) P_{k,n}^\dagger) U_n^\dagger) P_{k,n}^\dagger. \tag{3.28}$$

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

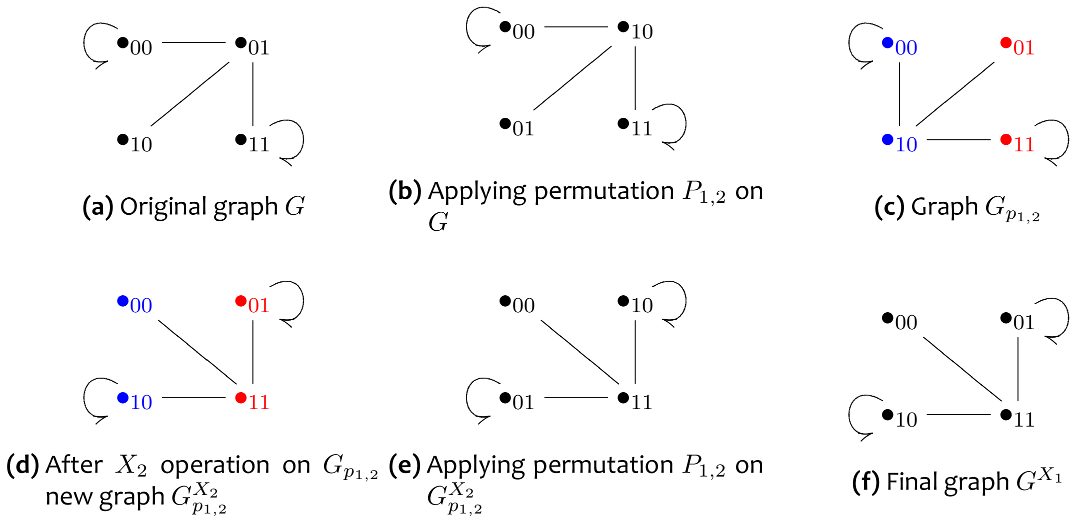
$$G \xrightarrow{p_{k,n}} G_{p_{k,n}} \xrightarrow{U_n} G_{p_{k,n}}^{U_n} \xrightarrow{p_{k,n}} G^{U_k} \tag{3.29}$$

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

Theorem 3.5. *Let G be a weighted undirected graph of order 2^n. Then $\rho(G^{U_k}) = U_k \rho(G) U_k^\dagger$ where $U_k = I_1 \otimes \cdots \otimes I_2 \otimes U \otimes I_2 \otimes \cdots \otimes I_2$, $k < n$ and $U \in \{X, Y, Z, H\}$ placed in the k-th position of the tensor product.*

Proof. Combining equation (3.27), (3.28) and (3.29) we find,

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



(a) Original graph G **(b)** Applying permutation $P_{1,2}$ on G **(c)** Graph $G_{p_{1,2}}$

(d) After X_2 operation on $G_{p_{1,2}}$ new graph $G_{p_{1,2}}^{X_2}$ **(e)** Applying permutation $P_{1,2}$ on $G_{p_{1,2}}^{X_2}$ **(f)** Final graph G^{X_1}

Figure 3.7 : X operation on the first qubit of a 2-qubit state

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

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

Hence proved. □

Example 3.5. *In the last theorem, instead of taking a general unitary operator U_k let us consider X_k, that is, an X gate operation on the k-th qubit. The theorem suggests the following steps:*

1. *Apply the permutation $P_{k,n}$ on the initial graph G to get graph $G_{p_{k,n}}$.*

2. *Now we construct $G_{p_{k,n}}^{X_n}$ from $G_{p_{k,n}}$ by applying the procedure 3.1.*

3. *We again apply $P_{k,n}$ on $G_{p_{k,n}}^{X_n}$ to get G^{X_k}.*

In a graph of four vertices representing a 2 qubit quantum state, we have seen graph switching for X gate operation on second qubit. Now we are able to discuss the X gate operation on first qubit. We have shown different steps of X_1 operation in sequence in the figure 3.7. One can easily check that $\rho(G^{X_1}) = X_1\rho(G)X_1$.

3.3.6 CNOT gate operation

The $CNOT$ gate occupies a central position in various quantum information processing tasks to generate non-locality and entanglement in quantum states as well as different quantum information and coding theoretic tasks. It is represented by the unitary matrix,

$$C_{NOT} = \begin{bmatrix} I & 0 \\ 0 & X \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \tag{3.30}$$

Note that, it acts on two qubit quantum states. A graph with four vertices represents a two qubit state. Thus, here we mention the graph switching method equivalent to CNOT gate applicable for graphs with four vertices.

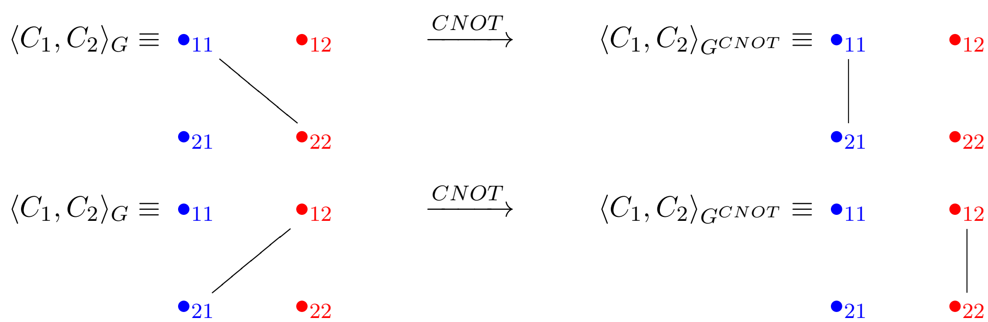
A graph of order 4, representing a 2-qubit quantum state consists of two cluters $C_\mu = \{v_{\mu,1}, v_{\mu,2}\}$ for $\mu = 1, 2$. Let G^{CNOT} be the graph generated from the graph G such that $\rho(G^{CNOT}) = C_{NOT}\rho(G)C_{NOT}^\dagger$. We generate G^{CNOT} by the following switching procedure.

Procedure 3.5. CNOT operation

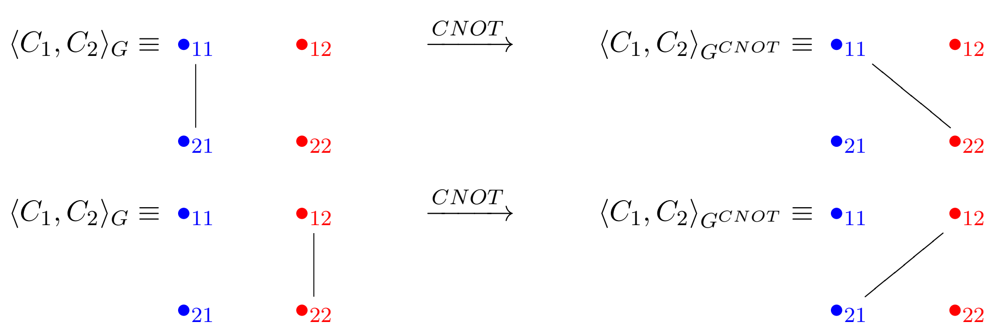
1. *The induced subgraph $\langle C_1\rangle$ will remain invariant in both G and G^{CNOT}.*

2. *The loops of $\langle C_2\rangle$ will interchange their position to generate G^{CNOT} from G.*

3. *If there is an edge joining two vertices of opposite colours in $\langle C_1, C_2\rangle_G$ then $\langle C_1, C_2\rangle_{G^{CNOT}}$ contains an edge joining different colors. Pictorially,*



4. *If there is an edge joining two vertices of same colour in $\langle C_2\rangle_G$ then $\langle C_2\rangle_{G^{CNOT}}$ contains an edge joining vertices of same colour. Pictorially,*



Theorem 3.6. *Let G be a graph of order 4 with two clusters, each containing two vertices. The graph G^{CNOT} is generated by the above procedure from the graph G. Then, $\rho(G^{CNOT}) = C_{NOT}\rho(G)C_{NOT}^\dagger$.*

Proof. Note that, $C_{NOT}\rho(G)C_{NOT}^\dagger = \frac{1}{d(G)}C_{NOT}(D(G) + A(G))C_{NOT}^\dagger = \frac{1}{d(G)}(C_{NOT}D(G)C_{NOT}^\dagger + C_{NOT}A(G)C_{NOT}^\dagger)$. Now,

$$C_{NOT}A(G)C_{NOT}^\dagger = \begin{bmatrix} I & 0 \\ 0 & X \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & X \end{bmatrix}^\dagger = \begin{bmatrix} IA_{11}I & IA_{12}X^\dagger \\ XA_{21}I & XA_{22}X^\dagger \end{bmatrix} = \begin{bmatrix} A_{11} & IA_{12}X^\dagger \\ XA_{21}I & XA_{22}X^\dagger \end{bmatrix}. \tag{3.31}$$

In the above equation, A_{11} represents the adjacency matrix of the subgraph $\langle C_1\rangle$ which remains invariant under the $CNOT$ operation. Also, A_{22} represents the adjacency matrix corresponding to the induced subgraph $\langle C_2\rangle$, which is converted to $XA_{22}X^\dagger$. Now, $XA_{22}X^\dagger$ is the X gate operation on $\langle C_2\rangle$, that is, interchange of the loops between the vertices. We also observe that the changes in the subgraph $\langle C_1, C_2\rangle$ is equivalent to the matrix operation

$$\begin{bmatrix} 0 & A_{12} \\ A_{21} & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 & IA_{12}X^\dagger \\ XA_{21}I & 0 \end{bmatrix}.$$

Combining we find that $C_{NOT}A(G)C_{NOT}^{\dagger} = A(G^{CNOT})$. Also, $(C_{NOT}D(G)C_{NOT}^{\dagger}) = D(G^{CNOT})$. Therefore, $C_{NOT}\rho(G)C_{NOT}^{\dagger} = \rho(G^{CNOT})$. $\square$

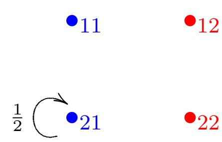
3.3.7 Bell state generation

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 [Adhikari et al., 2017], and is also discussed in Chapter 2.

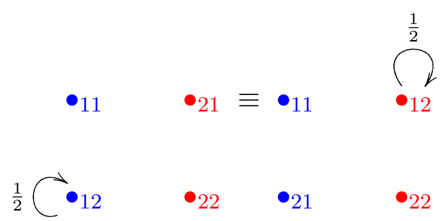
We begin with the initial state $|10\rangle$. We operate a Hadamard gate on the first qubit followed by a CNOT gate to generate Bell state as follows,

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

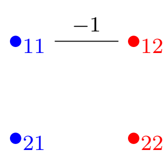
Graph, corresponding to state $|10\rangle\langle 10|$, with vertex decomposition $\mathcal{C} = C_1 \cup C_2$, is



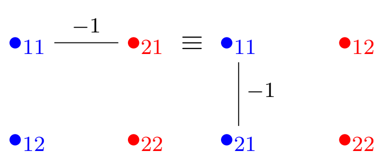
To apply Hadamard gate on first qubit, i.e., H_1, we first swap vertices. The graph changes to



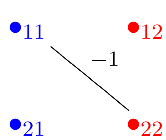
Apply H_2 and get a new graph



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



Now apply CNOT operation. Following the procedure discussed above, the new graph represents the state $\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$ [Adhikari et al., 2017].



Similarly, all other Bell states can be generated graph theoretically.

3.4 WHAT NEXT?

In this chapter, we have observed that familiar quantum grate operations has a graph theoretic counterpart. Therefore, graph theoretic operations can be used in quantum computation. There are a number of open problems in this direction. Some of them are mentioned below.

1. Let G and G_1 be two graphs such that $\rho(G)$ and $\rho(G_1)$ have equal eigenvalues. From the structure of the graphs we need to justify existence or non-existence of a unitary operator U such that $\rho(G_1) = U\rho(G)U^\dagger$.

2. Let there is a unitary operator U such that $\rho(G_1) = U\rho(G)U^\dagger$ holds. From the graph theoretic properties we need to justify whether U is a local or a global unitary operator.