2
Graph Theory and Quantum Information

There are many popular applications of graph theory in quantum mechanics and information theory. A Google search with "*quantum mechanics and graph theory*" received $6,89,000$ results 0.49 seconds. The properties of mixed quantum states derived from the graph Laplacian matrices is the fundamental concern of this thesis, which has its roots in a work in 2006 [Braunstein et al., 2006b]. In this chapter, we present a brief introduction to quantum information and graph theory, which will be of use in the later part of this work frequently. We assume a basic idea of linear algebra and matrix analysis [Horn and Johnson, 2012] as a prerequisite for this work.

2.1 AN INTRODUCTION TO QUANTUM INFORMATION THEORY

The characteristics of quantum states are essential ingredients in quantum information and computation. A quantum state is represented by a column vector belonging to a projective Hilbert space $\mathcal{H}^{(N)}$ of dimension N. For brevity, we may leave out the word "projective". Thus, from now on, Hilbert space will imply a projective Hilbert space. Following the standard nomenclature of quantum mechanics, we use Dirac's notation $|\psi\rangle$ to designate the state vector ψ. The conjugate transpose of $|\psi\rangle$ is denoted by $\langle\psi|$. Standard inner product of two state vectors $|\psi\rangle$ and $|\phi\rangle$ is denoted by $\langle\psi|\phi\rangle \in \mathbb{C}$. Also, $|\psi\rangle\langle\phi|$ is the outer product between $|\psi\rangle$ and $|\phi\rangle$, which is a complex square matrix.

In classical information and coding theory a binary digit or a bit is the basic unit of information. A bit has one of the two values either 0 or 1. The quantum information theoretic counterpart of a bit is the qubit. A quantum state in $\mathcal{H}^{(2)}$ is called a qubit. The standard basis of $\mathcal{H}^2$ is given by,

$$\left\{|0\rangle, |1\rangle : |0\rangle = \begin{pmatrix}1\\0\end{pmatrix}, |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}\right\}, \tag{2.1}$$

that is also called the computational basis. Thus, a qubit is represented by,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \text{ where } |\alpha|^2 + |\beta|^2 = 1, \text{ and } \alpha, \beta \in \mathbb{C}. \tag{2.2}$$

A qudit is a quantum state in higher dimension. In general, the computational basis of $\mathcal{H}^{(N)}$ is given by,

$$\{|d_i\rangle : |d_i\rangle = (0, 0, \ldots 1(i\text{-th position}), 0, \ldots 0)^\dagger\}. \tag{2.3}$$

Here, we use '$\dagger$' to indicate conjugate transpose. In general, a qudit is given by,

$$|\psi\rangle = \sum_i \alpha_i |d_i\rangle \text{ where } \sum_i |\alpha_i|^2 = 1, \text{ and } \alpha_i \in \mathbb{C}. \tag{2.4}$$

Definition 2.1. Pure and mixed state: *A quantum system is in a pure state if it can be represented with a single state vector $|\psi\rangle$. If a quantum system has different states $|\psi_i\rangle$ with probability p_i, then we call the state a mixed state. We may represent a mixed quantum system as an ensemble of pure state $\{p_i, |\psi_i\rangle\}$.*

An alternative representation of quantum state uses the idea of density matrix. Mathematically the idea of state vector and the density matrix is equivalent. But, the density matrix approach is more convenient for dealing with mixed states and we use throughout the thesis. In general we utilize this idea throughout the thesis. An ensemble $\{p_i, |\psi_i\rangle\}$ can be used to represent a density matrix as,

$$\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|, \text{ where } p_i > 0 \text{ and } \sum_i p_i = 1. \tag{2.5}$$

The general definition of a density matrix is given below:

Definition 2.2. Density matrix: *A density matrix ρ is a positive semi-definite Hermitian matrix with unit trace.*

In terms of density matrix, we can classify pure and mixed quantum states. A quantum system represented by a density matrix ρ is in a pure state if there is a state vector $|\psi\rangle$ such that $\rho = |\psi\rangle \langle\psi|$. Otherwise, the state is a mixed state that is a convex combination of pure states, as represented in the above equation.

Different characteristics of pure and mixed states are discussed in literature [Barnett, 2009]. Recall that, given any state vector $|\psi\rangle$, the outer product $|\psi\rangle \langle\psi|$ is a rank one Hermitian positive semi-definite matrix. Also, the convex combination of positive semi-definite Hermitian matrices is again a positive semi-definite Hermitian matrix. Using this property we may identify density matrices of pure and mixed states. In brief, we may write:

Lemma 2.1. *A density matrix ρ represents a pure state if and only if rank of $\rho = 1$.*

The Kronecker product is the best natural notation of a product for states living in different spaces. We have mentioned that the space associated to quantum states is a Hilbert space $\mathcal{H}$. Quantum states are rays in $\mathcal{H}$. In quantum mechanics, we want every action of an operator on the individual state to define an action on the combined or product state. The Kronecker product is exactly that. Given two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ and linear map $T_i : \mathcal{H}_i \to \mathcal{H}_3$, the product space, we have a bilinear map $(T_1, T_2) : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathcal{H}_3$. Corresponding to this bilinear map there is a unique linear map, $T_1 \otimes T_2 : \mathcal{H}_1 \otimes \mathcal{H}_2 \to \mathcal{H}_3$ which is the Kronecker product. We define it as follows.

Definition 2.3. Kronecker product: *The Kronecker product [Van Loan, 2000] of two matrices $A = (a_{ij})_{m\times m}$ and $B = (b_{ij})_{n\times m}$ is denoted by $A \otimes B$ and defined by $A \otimes B = (a_{ij}B)_{mn\times mn}$.*

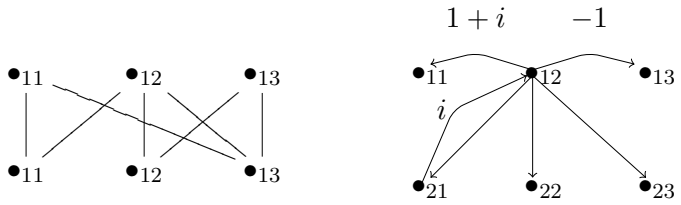
Similarly, given two vectors $|\phi\rangle = (\phi_1, \phi_2, \ldots \phi_m) \in \mathcal{H}^{(m)}$ and $|\psi\rangle = (\psi_1, \psi_2, \ldots \psi_n) \in \mathcal{H}^{(n)}$ we define the Kronecker product $|\phi\rangle \otimes |\psi\rangle = (\phi_1 |\psi\rangle, \phi_2 |\psi\rangle, \ldots \phi_m |\psi\rangle)$. In short, we denote it as $|\phi\psi\rangle$. Also the product Hilbert space $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$ is defined by,

$$\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)} = \left\{ |\psi\rangle \otimes |\phi\rangle : |\psi\rangle \in \mathcal{H}^{(m)}, |\phi\rangle \in \mathcal{H}^{(n)} \right\}. \tag{2.6}$$

Similarly, the product of k spaces $\mathcal{H}^{(n_i)}, i = 1, 2, \ldots k$ as follows:

$$\bigotimes_{i=1}^{k} \mathcal{H}^{(n_i)} = \left\{ |\psi_1\rangle \otimes |\psi_2\rangle \otimes \ldots |\psi_k\rangle : |\psi_i\rangle \in \mathcal{H}^{(n_i)} \right\}. \tag{2.7}$$

It is easy to check that given vectors spaces, $\mathcal{H}^{(n_i)} : i = 1, 2, \ldots k$, the product space $\otimes_i \mathcal{H}^{(n_i)}$ is also a Hilbert space.



(a) Simple graph **(b)** Weighted digraph

Figure 2.1 : Examples of simple and weighted digraphs

A quantum state belongs to $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$ is called a bipartite quantum state. A multipartite quantum state belongs to $\bigotimes_{i=1}^{k} \mathcal{H}^{(n_i)}$. We have mentioned earlier that a state in $\mathcal{H}^{(2)}$ is called a qubit. In a similar fashion, we call a states in $\mathcal{H}^{(2)} \otimes \mathcal{H}^{(2)}$ two qubit state. In general, a state in $\bigotimes_{i=1}^{k} \mathcal{H}_i^{(2)}$ is called a k-qubit state.

This provide the minimal terminology on quantum information theory needed for the thesis. More information will be discussed as and when required.

2.2 FROM GRAPH THEORY TO QUANTUM INFORMATION

Here, we clarify the connection between combinatorial graphs [West, 2001] and the density matrices of the quantum state, in which we are interested. We begin with a brief introduction to graph theory needed for this thesis. Then, we introduce *Graph Laplacian states*.

2.2.1 Essential terminologies of graph theory

A graph $G = (V(G), E(G))$ consists of a vertex set $V(G)$ and an edge set $E(G) \subset V(G) \times V(G)$. Order of a graph is given by the number of its vertices. The directed edge $\hat{e} = (u, v)$ is called an outgoing edge from the vertex u and an incoming edge to the vertex v. A loop (u, u) is an edge which starts and ends at the vertex u. A graph with directed edges is called digraph. The edge weight function of G is a mapping $w_G : V(G) \times V(G) \to \mathbb{C}$ defined by,

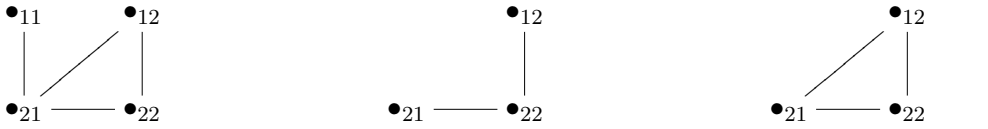
$$w_G(u, v) = \begin{cases} w_{u,v} & \text{if } (u, v) \in E(G), \\ 0 & \text{if } (u, v) \notin E(G). \end{cases} \tag{2.8}$$

If edge weight is not specified we assume it one. A graph with multiple weighted directed edges between two vertices is called a weighted multi-digraph. A weighted multi-digraph is shown in the figure 2.1b. We call a graph as empty graph if it has an empty edge set.

A simple graph is a special case of weighted multi-digraph which consists of undirected edges. An undirected edge $e = (u, v)$ is a combination of two oppositely oriented directed edges $\hat{e}_1 = (u, v)$ and $\hat{e}_2 = (v, u)$. Thus, if $(u, v) \in E(G)$ then $(v, u) \in E(G)$. Also, a simple graph has no loop. Edge weight of its edges are 1. A simple graph is shown in figure 2.1a.

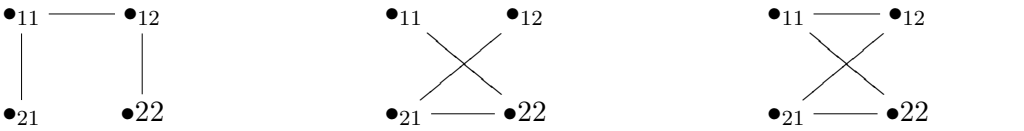
Definition 2.4. Subgraph: *A graph H is said to be a subgraph of a graph G, if $V(H) \subset V(G)$ and $E(H) \subset E(G)$. Also the weight function w_H is a restriction of w_G on $E(H)$.*

Definition 2.5. Induced subgraph: *A subgraph H is an induced subgraph of the graph G provided given $u, v \in V(H)$ and $(u, v) \in E(G)$ indicates $(u, v) \in E(H)$.*



(a) Graph **(b)** A subgraph **(c)** An induced subgraph

Figure 2.2 : A subgraph and an induced subgraph of a graph



(a) A graph G **(b)** Isomorphic copy of G **(c)** Graph non-isomorphic to G

Figure 2.3 : Isomorphic and non-isomorphic copy of a graph

A subgraph is a part of a graph, widely used in graph theoretical applications. In the figure 2.2 we depict an examples of a subgraph and an induced subgraph.

Graph isomorphism problem is an important problem in graph theory and network analysis and is defined as follows:

Definition 2.6. Graph Isomorphism: *Two graphs G and H are isomorphic if there is a bijective function $f : V(G) \to V(H)$ such that $(u, v) \in E(G) \Leftrightarrow (f(u), f(v)) \in E(H)$, as well as, $w_G(u, v) = w_H(f(u), f(v))$.*

For simple graphs, weights of every edge is one and we neglect condition on edge weight. Two isomorphic graphs have equal number of vertices and edges. Also, they have same strectural properties such as chromatic number, spectral values, degree sequence etc. In this thesis, we call two graphs G and H are equal if they are isomorphic with the identity mapping i acting as the graph isomorphism.

Example 2.1. *Consider the graph G in the figure 2.3(a) and H 2.3(b). This graph isomorphism is lead by the bijective mapping $f : V(G) \to V(H)$ where $f(v_{11}) = v_{21}, f(v_{12}) = v_{22}, f(v_{21}) = v_{12}, f(v_{22}) = v_{11}$. But the graph in the figure 2.3(c) is not isomorphic to 2.3(a) as it has an additional edge.*

2.2.2 Basic assumptions on graphs

Graph theory and quantum mechanics are two different branches of science. The aim of this thesis is to illuminate the interface of these two distinct subjects. The interaction between them depends on a number of assumptions. For the development of the combinatorial visualization of quantum states we need the following hypothesis on all the graphs used in this thesis.

Assumption 2.1. Basic assumptions:

1. *Given any directed edge $\hat{e} = (u, v) \in E(G)$ there is an edge of opposite orientation $(v, u) \in E(G)$.*
2. *The edge weight function satisfies the property $w(u, v) = \overline{w(v, u)}$, where $\overline{w(v, u)}$ is the complex conjugate of $w(v, u)$.*
3. *For any vertex u there may be at most one loop with non-negative real weight r_u.*

Existence of an undirected edge (u,v) indicates two directed edges of opposite orientations (u, v) and (v, u) in $E(G)$. If weight of all the undirected edges is 1 then $w(u, v) = \overline{w(v, u)} = 1$. Therefore, a simple graph follows the basic assumptions. From now on we shall consider only those graphs which satisfies these assumptions. The first assumption states existence of two oppositely oriented edges (u, v) and (v, u). Therefore for simplicity, instead of drawing two directed edges (u, v) and (v, u) we shall draw one undirected edge (u, v).

2.2.3 Matrices related to graphs

Spectral graph theory is an interesting branch of graph theory. Graph spectra revels fundamental properties of graphs. It links the discrete mathematics to the continuous one through algebraic, geometric and analytic techniques. In spectral graph theory, we study a number of matrices corresponding to a given graph. Foundation of this thesis needs the definitions of adjacency matrix, Laplacian and the signless Laplacian matrices related to weighted digraphs which we shall discuss now [Adhikari et al., 2017].

A graph consists of vertices and edges. Two vertices are adjacent if they are connected by an edge. This adjacency relation between vertices is represented by a matrix, which is the adjacency matrix, defined below for weighted graph:

Definition 2.7. Adjacency matrix: *The adjacency matrix $A(G) = (a_{uv})$ associated to G is defined as*

$$a_{uv} = \begin{cases} w_{uv}, & \text{if } (u, v) \in E; \\ \overline{w}_{uv}, & \text{if } (v, u) \in E; \\ r_u, & \text{if } (u, u) \in E; \\ 0, & \text{otherwise.} \end{cases}$$

Degree of a vertex represents connectivity, and importance of a vertex in a graph. Vertex degree and degree matrix is defined as follows:

Definition 2.8. Degree of a vertex: *The weighted degree d_u of a vertex $u \in V$ is given by $d_u = \sum_{v=1}^{n} |a_{uv}|$.*

Definition 2.9. Degree matrix: *The degree matrix of a graph is a diagonal matrix $D(G) = \text{diag}\{d_u : u \in V(G)\}$.*

Definition 2.10. Degree of a graph: *Also degree of a graph $d(G)$ is the sum of all the vertex degrees. In short, $d(G) = \text{trace}(D(G))$.*

A regular graph has equal degree for all the vertices. Let G be a regular graph of order n. The degree of its vertices is r. Then the degree matrix is $D(G) = rI_n$, where I_n is the identity matrix of order n. A complete graph has all possible edges. In a simple graph of order n, an individual vertex may be connected to maximum $(n - 1)$ other vertices. Therefore, in a complete simple graph degree of every vertices is $(n - 1)$. Hence, complete graph is a regular graph such that $D(G) = (n - 1)I_n$.

The idea of Laplacian operator originally belongs to partial differential equations where it is useful for studying, for example, energy flow in a system. In spectral graph theory, the Laplacian matrix is its discrete counterpart. It can be used for investigating energy flow in a network. In our work we use it to generate quantum density matrices corresponding to a graph.

Definition 2.11. Laplacian and the signless Laplacian matrices: *The Laplacian and the signless Laplacian matrices are defined by $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$, respectively.*

Every vertex of the graph represents a row and a column of the above matrices. Thus, order of these matrices is the number of vertices in the graph. For simple graphs the above definitions take a more simplified form under the assumption, $w_{uv} = w_{vu} = 1$ and $r_{u,v} = 0$. Thus, the adjacency matrix $A(G) = (a_{ij})$ for a simple graph G is given by,

$$a_{uv} = \begin{cases} 1 & \text{if } (u,v) \in E; \\ 0, & \text{otherwise.} \end{cases} \tag{2.9}$$

Also, degree of a vertex u becomes the number of edges adjacent to it. Degree matrix contains vertex degrees in the diagonal. If $L = (l_{uv})$ and $Q = (q_{uv})$ be Laplacian and signless Laplacian matrices of a graph, then

$$l_{uv} = \begin{cases} -1 & \text{if } (u,v) \in E \text{ and } u \neq v; \\ d_u & \text{if } u = v; \\ 0, & \text{otherwise;} \end{cases}, \text{ and } q_{uv} = \begin{cases} 1 & \text{if } (u,v) \in E \text{ and } u \neq v; \\ d_u & \text{if } u = v; \\ 0, & \text{otherwise;} \end{cases}. \tag{2.10}$$

Algebraic properties of adjacency, Laplacian and signless Laplacian matrices are reviewed in [Bapat, 2010; Merris, 1998; Cvetković and Simić, 2009, 2010a,b]. Below we mention a number of useful properties of these matrices under the basic assumptions 2.1 on graphs:

1. The matrices $A(G), D(G), L(G)$, and $Q(G)$ are Hermitian matrices. Recall that a matrix M is Hermitian if $M^\dagger = M$.

2. The Laplacian matrices $L(G)$ and $Q(G)$ are positive semi-definite matrices. A matrix M is positive semi-definite if its eigenvalues are non-negative.

3. If the graphs G and H be isomorphic then there is a permutation matrix P such that $A(H) = PA(G)P^\dagger$, $L(H) = PL(G)P^\dagger$, and $Q(H) = PQ(G)P^\dagger$ holds simultaneously.

The above properties are essential in this thesis. Property 1 and 2 will be applicable for defining density matrices. The point 3 has bidirectional significance in our work. It assures that the adjacency matrix and the Laplacian matrices of two isomorphic graphs have equal spectra. But, the converse is not true. Therefore, an interesting task in graph theory is to collect classes of non-isomorphic graphs of equal spectra. We have provided a method for constructing such graphs in Chapter 6. In Chapter 4, we have utilized graph isomorphism as a global unitary operator to generate entanglement using mixed quantum states.

2.2.4 Graph Laplacian quantum states and their properties

Now we are in position to discuss the connection between graphs and density matrices representing quantum states. Recall that density matrix of a quantum state is a positive semi-definite Hermitian matrix with unit trace.

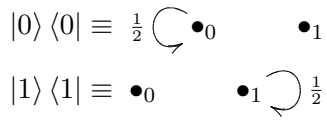


Figure 2.4 : Qubits $|0\rangle$ and $|1\rangle$ as graphs.

Definition 2.12. Graph Laplacian quantum states: *A graph Laplacian quantum state is represented by a density matrix of the form,*

$$\rho_l(G) = \frac{L(G)}{\text{trace}(L(G))} \text{ or } \rho_q(G) = \frac{Q(G)}{\text{trace}(Q(G))},$$

where $L(G)$ and $Q(G)$ are Laplacian and signless Laplacian matrix of the graph, respectively. If no confusion occurs we may denote $\rho_l(G)$ and $\rho_q(G)$ together with $\rho(G)$.

Note that, trace$(L(G))$ = trace$(Q(G))$ = trace$(D(G)) = d$, degree of the graph. The above definition indicates, if $\rho(G) = (\rho_{uv})$ then

$$\rho_{uv} = \begin{cases} s\frac{w_{uv}}{d} & \text{if } u \neq v \text{ and } (u,v) \in E(G), \\ 0 & \text{if } u \neq v \text{ and } (u,v) \notin E(G), \\ \frac{d_u}{d} & \text{if } u = v. \end{cases} \tag{2.11}$$

Here $s = 1$ for $\rho(G) = \rho_q(G)$ and $s = -1$ for $\rho(G) = \rho_l(G)$. If G be a simple graph, then $w_{uv} = 1$ in the above equation.

Note that, $L(G)$ and $Q(G)$ depend on the vertex labelling of the graph. Hence, two isomorphic copies of a graph represent two different quantum states. Properties of these two quantum states differ significantly. Moreover, there is a graph Laplacian quantum state corresponding to every graph but the converse is not true. In theorem 2.1, we present a necessary and sufficient condition for a quantum state to be a graph Laplacian quantum state. Before that we present an example and a counter example.

Example 2.2. *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 shown in the figure 2.4. These graphs do not have any edge but have a loop of weight $\frac{1}{2}$.*

Example 2.3. *Consider the quantum state*

$$\rho = \frac{1}{5}|0\rangle\langle 0| + \frac{2}{5}|0\rangle\langle 1| + \frac{2}{5}|1\rangle\langle 0| + \frac{4}{5}|1\rangle\langle 1| = \frac{1}{5}\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}.$$

We claim that this quantum state is not graphical, which will be justified in theorem 2.1. Note that, in this case, $\rho_{11} \leq \rho_{12}$.

We need the definition of diagonally dominant matrix [Horn and Johnson, 2012] before stating theorem 2.1. These matrices have a number of interesting properties which are useful in our work. A Hermitian diagonally dominant matrix, whose diagonal entries are non-negative real number, is always positive semidefinite.

Definition 2.13. Diagonally dominant matrix: *A matrix $A = (a_{ij})_{N\times N}$ is said to be diagonally dominant if $|a_{ii}| \geq \sum_{j=1, j\neq i}^{N} |a_{ij}|$ for all $i = 1, 2, \ldots N$.*

Theorem 2.1. *A quantum state ρ is a graph Laplacian state if and only if it is a diagonally dominant matrix.*

Proof. Let order of the matrix ρ be N. If ρ has a graph representation, the weighted digraph G has N vertices. When $i \neq j$ and $\rho_{ij} \neq 0$ there is a directed edge (i, j) with edge weight $w(i, j) = \rho_{ij}$. As ρ is a positive semi-definite Hermitian matrix, $\rho_{ji} = \overline{\rho_{ij}}$. Thus (i, j) and (j, i) exists togther with $w(j, i) = \overline{w(i, j)}$. Also as ρ is a positive semi-definite Hermitian matrix, all the diagonal entries ρ_{ii} is a non-negative real number. Besides, $\rho_{ii} = d_i + sa_{ii}$. Here $s = -1$ for $\rho_l(G)$ and $s = 1$ for $\rho_q(G)$. Now,

$$\begin{aligned}\rho_{ii} =& d_i + sa_{ii} = \sum_{j=1}^{N} |w(i, j)| + sw(i, i) = \sum_{j\neq i} |w(i, j)| + |w(i, i)| + sw(i, i) \\ =& \sum_{j\neq i} |\rho_{ij}| + |w(i, i)| + sw(i, i).\end{aligned} \tag{2.12}$$

As ρ_{ii} is real, $w(i, i)$ must be real in the above expression. Two cases arise.

- Case-I: Let $w(i, i) = 0$ or $|w(i, i)| = -sw(i, i)$. In any case, $\rho_{ii} = \sum_{j\neq i} |\rho_{i,j}|$.
- Case-II: Let $w(i, i) \neq 0$ and $|w(i, i)| + sw(i, i) = 2|w(i, i)|$. Then, from the above equation,

  $$|w(i, i)| = \frac{\rho_{ii} - \sum_{i\neq j} |\rho_{ij}|}{2} \geq 0. \tag{2.13}$$

  In this case, $\rho_{ii} \geq \sum_{i\neq j} |\rho_{ij}|$.

Combining them we come to the conclusion. □

2.2.5 Revisit pure and mixed states

Now we like to recall the definition 2.1 of pure and mixed states. Pure states is represented by a state vector. A mixed quantum state, on the other hand, requires an ensemble of pure states or a density matrix with rank > 1. In practice a mixed quantum state is much more likely to occur as interaction with the ambient environment causes a pure state to becomes mixed. Various types of noises occur when we try to transmit a pure quantum state via a channel. Thus, studying properties of mixed quantum states is crucial in quantum mechanics and information. Before going to the detailed study of Graph Laplacian quantum states we should state some conditions to classify pure and mixed states.

A vertex is an isolated vertex in a graph if it is not connected to any other vertex with an edge. Thus degree of an isolated vertex is zero. Also the row and the column corresponding to an isolated vertex consists of zeros only. Thus, existence of isolated vertex reduce the rank of the density matrix in a graph. Recall that, a density matrix of a pure state is a rank one matrix. Another characteristics of rank of a square matrix follows from number of its non-zero eigenvalues. Rank of the matrix is equal to the number of non-zero eigenvalues of the matrix. Rank one density matrices corresponding to a few classes of graphs. The following result holds for simple graphs.

Theorem 2.2. *The density matrix of a simple graph G is pure if and only if $G = K_2$ or $G = K_2 \sqcup v_1 \sqcup v_2 \ldots v_l$, for some isolated vertices $v_1, v_2, \ldots, v_l$. [Braunstein et al., 2006b]*

Here K_2 is the complete graph consisting of two vertices and an edge joining them. Thus, G consists of only one edge and all disjoint vertices. This result was generalized in [Adhikari et al., 2017] for directed graphs with loops. Let O_1 represents a graph with only one vertex having a weighted loop. Adding some additional isolated vertices with it we get a new graph $\hat{O}_1 = O_2 \sqcup v_1 \sqcup v_2 \ldots v_l$. Several examples of well known pure states are shown in the next section.

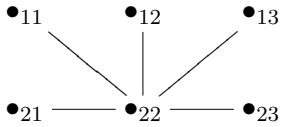


Figure 2.5 : A star graph which corresponds to a state in $\mathcal{H}^{(2)} \otimes \mathcal{H}^{(3)}$.

Theorem 2.3. *Let G be a weighted digraph with loops having non-negative weights and is isomorphic to $\hat{O}_1$. Then $\rho_q(G)$ defined by the signless Laplacian of G represents a pure state [Adhikari et al., 2017].*

These above two results show that the class of graphs representing pure quantum states is very limited. In general, a graph consists of more than one loop or edge. Thus, graph Laplacian quantum states are mixed, in general. Therefore, they provide a platform for studying properties of a broad class of mixed quantum states, where we utilize well established graph theoretic techniques. Consider the following example.

Example 2.4. *Let us consider a star graph of order 6 depicted in the figure 2.5. The density matrices corresponding to Laplacian and signless Laplaocian matrices are given by,*

$$\rho_l(G) = \frac{1}{10}\begin{bmatrix} 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 1 & -1 & -1 & -1 & 5 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{bmatrix}, \text{ and } \rho_q(G) = \frac{1}{10}\begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 5 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

One may easily check that the above density matrices represents mixed quantum states. Quantum states related to star graphs have many important properties, studied in literature. All of them are entangled irrespective of vertex labellings due to their particular combinatorial structure [Braunstein et al., 2006b].

2.2.6 Relation between clustering on the vertex set and Hilbert spaces

In the last subsection, we have defined the Graph Laplacian quantum states and stated conditions for a quantum state to be in this class. Recall that, a density matrix acts on a Hilbert space, which may have a tensor product structure. For example a density matrix ρ of order 4 may represent a state in $\mathcal{H}^{(4)}$ or $\mathcal{H}^{(2)} \otimes \mathcal{H}^{(2)}$. When we deal with density matrices, the underlined Hilbert space should be clarified from the graph.

Let a graph Laplacian quantum state in $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$ be represented by the density matrix ρ corresponding to the graph G with N vertices. Then, $N = m \times n$. We partition the vertex set into m disjoint clusters each containing n vertices as follows.

$$\begin{aligned} &V = C_1 \cup C_2 \cup \cdots \cup C_m; \\ &C_\mu \cap C_\nu = \emptyset \text{ for } \mu \neq \nu \text{ and } \mu, \nu = 1, 2, \ldots m; \\ &C_\mu = \{v_{\mu 1}, v_{\mu 2}, \ldots v_{\mu n}\}. \end{aligned} \tag{2.14}$$

For any vertex $v_{\mu i}$, the Roman index i represents the position of a vertex in μ-th cluster which is indexed by a Greek index. The clustering arrange the graphs as a two dimensional grid graph as depicted in the figure 2.6. Also it partitions all corresponding matrices into blocks. Below we

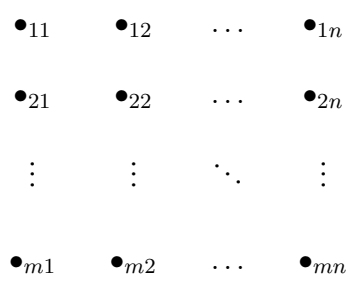


Figure 2.6 : Grid structure of the vertex set after clustering.

constitute the adjacency matrix as a block matrix.

$$A(G) = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{bmatrix}_{N\times N}, \tag{2.15}$$

where $A_{\mu\nu}$ are blocks of order $n \times n$ [Dutta et al., 2016b]. As $A(G)$ is a Hermitian matrix, we have $A^\dagger_{\mu\mu} = A_{\mu\mu}$ and $A^\dagger_{\mu\nu} = A_{\nu\mu}$, for $\mu \neq \nu$. The induced subgraph generated by C_μ is denoted by $\langle C_\mu\rangle$. Note that, the adjacency matrix of the subgraph $\langle C_\mu\rangle$ is given by the block $A_{\mu\mu}$. For $\mu \neq \nu$, the subgraph generated by the vertex set $C_\mu \cup C_\nu$ and all the edges $\{(u, v) : u \in C_\mu, v \in C_\nu\}$ is denoted by $\langle C_\mu \cup C_\nu\rangle$. The block $A_{\mu\nu}$ gives the adjacency relations in the graph $\langle C_\mu \cup C_\nu\rangle$. The adjacency matrix of $\langle C_\mu \cup C_\nu\rangle$ is

$$A(\langle C_\mu \cup C_\nu\rangle) = \begin{bmatrix} 0 & A_{\mu\nu} \\ A^\dagger_{\mu\nu} & 0 \end{bmatrix}. \tag{2.16}$$

Similarly, the Laplacian and signless Laplacian matrix and their corresponding density matrices are also partitioned into blocks.

Let the computational basis of $\mathcal{H}^{(m)}$ and $\mathcal{H}^{(n)}$ be $\{|\mu_a\rangle\}$ and $\{|\mu_b\rangle\}$, respectively. Also $E_{\mu\nu} = |\mu_a\rangle\langle\nu_a|$, and $B_{\mu,\nu} = \text{trace}_a[(|\mu_a\rangle\langle\nu_a| \otimes I_b)\rho]$, where I_b is the identity matrix acting on $\mathcal{H}^{(n)}$. A bipartite quantum state ρ acting on $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$ can be represented as,

$$\rho = \sum_{\mu,\nu} E_{\mu\nu} \otimes B_{\mu\nu}. \tag{2.17}$$

If we partition the density matrix $\rho_{mn\times mn}$ into m^2 blocks of order n then $B_{\mu\nu}$ would be the blocks of ρ. Now considering the graph representation of ρ we may construct the following relations between $B_{\mu\nu}$ and $A_{\mu,\nu}$

$$B_{\mu\nu} = \begin{cases} s\frac{A_{\mu\nu}}{d} & \text{if } \mu \neq \nu \\ \frac{D_\mu + sA_{\mu\mu}}{d} & \text{if } \mu = \nu, \end{cases} \tag{2.18}$$

where $s = 1$ for $\rho_q(G)$ and $s = -1$ for $\rho_l(G)$.

For simplicity, a multipartite system may also be represented by a number of bipartite systems. Some specifications help us to assume them as a bipartite system, which fulfil our needs. As an example, consider n-qubit quantum states, which belongs to the Hilbert space $\mathbb{C}^{(2)} \otimes \mathbb{C}^{(2)} \otimes \cdots \otimes \mathbb{C}^{(2)}$($n$-times). It may be considered as a bipartite system $\mathcal{H}_A \otimes \mathcal{H}_B$, where $\mathcal{H}_A = \mathbb{C}^{(2)} \otimes \mathbb{C}^{(2)} \otimes$

$\cdots \otimes \mathbb{C}^{(2)}(n-1)$ times) and $\mathcal{H}_B = \mathbb{C}^{(2)}$. An n-qubit quantum state is given by a density matrix of order 2^n. Hence, the density matrix $\rho(G)$ corresponding to a graph G with 2^n vertices represents an n-qubit quantum state. we consider a partitions of the vertex set

$$V(G) = \cup_{\mu=1}^{2^{n-1}} C_\mu, \tag{2.19}$$

where $C_\mu = \{v_{\mu,1}, v_{\mu,2}\}$. Then from the equation (2.15) we write,

$$\begin{aligned} A_{\mu,\mu} &= \begin{bmatrix} w(v_{\mu,1}, v_{\mu,1}) & w(v_{\mu,1}, v_{\mu,2}) \\ w(v_{\mu,2}, v_{\mu,1}) & w(v_{\mu,2}, v_{\mu,2}) \end{bmatrix}_{2\times 2} = \begin{bmatrix} w(v_{\mu,1}, v_{\mu,1}) & w(v_{\mu,1}, v_{\mu,2}) \\ w(v_{\mu,1}, v_{\mu,2}) & w(v_{\mu,2}, v_{\mu,2}) \end{bmatrix}_{2\times 2} \\ \text{and } A_{\mu,\nu} &= \begin{bmatrix} w(v_{\mu,1}, v_{\nu,1}) & w(v_{\mu,1}, v_{\nu,2}) \\ w(v_{\nu,2}, v_{\mu,1}) & w(v_{\mu,2}, v_{\nu,2}) \end{bmatrix}_{2\times 2} = \begin{bmatrix} w(v_{\mu,1}, v_{\nu,1}) & w(v_{\mu,1}, v_{\nu,2}) \\ w(v_{\mu,1}, v_{\nu,2}) & w(v_{\mu,2}, v_{\nu,2}) \end{bmatrix}_{2\times 2}. \end{aligned} \tag{2.20}$$

The above equations will come into use when we shall consider n qubit systems.

2.3 GRAPH STRUCTURE OF SOME QUANTUM STATES

In this section, we provide weighted digraphs whose density matrices represent a graph Laplacian quantum state having potential applications in quantum information and computation. Facets of quantum correlations such as entanglement, discord are useful resources. For the time being we consider them as properties of quantum states. Their formal definitions will be stated in later chapters.

2.3.1 Two qubit entangled states and Bell States

We have mentioned earlier that the simplest quantum state used in quantum information theory is a qubit. The minimal bipartite system consists of two qubits. A two qubit entangled quantum state is represented by,

$$|\psi\rangle = a\,|00\rangle + b\,|11\rangle\,, \tag{2.21}$$

where $a, b \in \mathbb{C} \setminus \{0\}$, and $|a|^2 + |b|^2 = 1$. Their density matrices are given by,

$$|\psi\rangle\langle\psi| = \frac{1}{2}\begin{bmatrix} |a|^2 & 0 & 0 & a\bar{b} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \bar{a}b & 0 & 0 & |b|^2 \end{bmatrix}. \tag{2.22}$$

The density matrix associated with G is given by any of $\rho_l(G)$ or $\rho_q(G)$. Consider the graph in Figure 2.7a. The graph has two loop of weight $|a|^2 - |ab|$, and $|b|^2 - |ab|$ on the vertices v_{11}, and v_{22}, respectively, as well as an edge of weight $w(v_{11}, v_{22}) = a\bar{b}$.

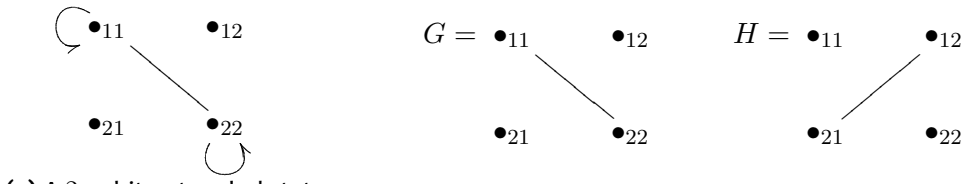
Bell states [Einstein et al., 1935; Bell, 1964] are maximally entangled two qubit states. We use them in bipartite quantum teleportation, dense coding and cryptography [Nielsen and Chuang, 2002]. They are represented as

$$|\phi^\pm\rangle = \frac{1}{\sqrt{2}}\,|00\rangle \pm |11\rangle\,, \text{ and } |\psi^\pm\rangle = \frac{1}{\sqrt{2}}\,|01\rangle \pm |10\rangle\,. \tag{2.23}$$

The corresponding density matrices are given by,

$$|\phi^\pm\rangle\langle\phi^\pm| = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & \pm 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \pm 1 & 0 & 0 & 1 \end{bmatrix} \text{ and } |\psi^\pm\rangle\langle\psi^\pm| = \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & \pm 1 & 0 \\ 0 & \pm 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{2.24}$$

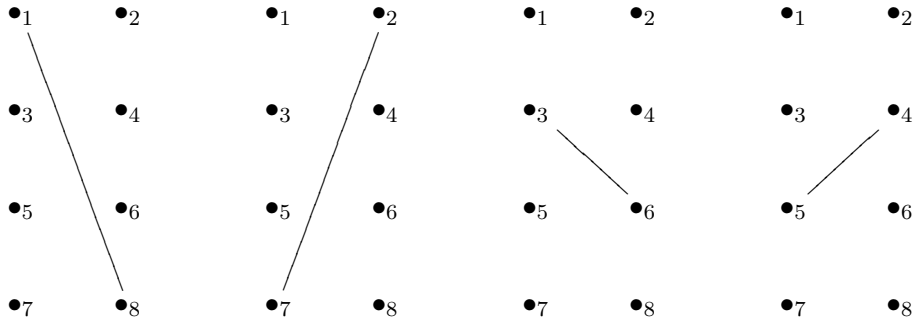
These density matrices corresponding to the following graphs G and H, respectively are depicted in Figure 2.7b. We may generalize them in higher dimension, adding more isolated vertices.



(a) A 2-qubit entangled state

(b) Bell states

Figure 2.7 : 2-qubit entangled states



(a) $|\psi\rangle^{(1,8)}$ **(b)** $|\psi\rangle^{(2,7)}$ **(c)** $|\psi\rangle^{(3,6)}$ **(d)** $|\psi\rangle^{(4,5)}$

Figure 2.8 : 3 qubit GHZ states

2.3.2 Three-qubit GHZ States

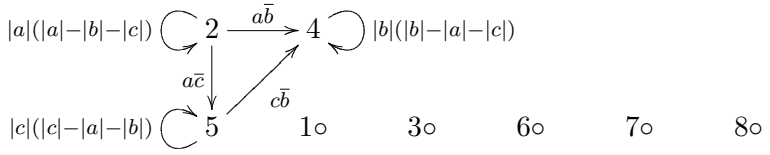
We apply three qubit quantum states when we involve three parties in a quantum information theoretic task. There are two classes of three qubit pure entangled states: W class and GHZ class [Greenberger et al., 1990; Dür et al., 2000]. Graph theoretic representation of W class states need some additional settings which will be stated in the next subsection. The eight orthogonal GHZ states are,

$$\begin{aligned} |\psi\rangle^{(1,8)} &= \frac{1}{\sqrt{2}}|000\rangle \pm |111\rangle\,, \qquad |\psi\rangle^{(2,7)} = \frac{1}{\sqrt{2}}|001\rangle \pm |110\rangle\,; \\ |\psi\rangle^{(3,6)} &= \frac{1}{\sqrt{2}}|010\rangle \pm |101\rangle\,, \qquad |\psi\rangle^{(4,5)} = \frac{1}{\sqrt{2}}|011\rangle \pm |100\rangle\,. \end{aligned} \tag{2.25}$$

We may represent their graphs as $\rho_l(G)$ or $\rho_q(G)$. The graphs corresponding to Equation (2.25) are given in Figures 2.8. They consists of one edge and isolated vertices. In higher dimensions they can be represented in a similar manner but with more isolated vertices.

2.3.3 Quantum states with signed Laplacian matrices

In [Adhikari et al., 2017] a new Laplacian matrix called signed Laplacian matrix was introduced. The density matrix for these classes of states can be expressed as $\frac{L_-(G)}{\text{trace}(L_-(G))}$, where $L_-(G)$



(a) 3 qubit W state in general

(b) 3 qubit W states for specific parameter values

Figure 2.9 : 3 qubit W states

is the signed Laplacian matrix of G. Like all other Laplacian matrices, $L_{-}(G)$ is also a positive semi-definite Hermitian matrix. In this case a graph representing a pure state may have multiple weighted directed edges and loops. Using it we represent the following quantum states, without going to further details.

The general three-qubit W state is given by $|\psi\rangle_{123}^{W} = a\,|001\rangle + b\,|010\rangle + c\,|100\rangle$ where $|a|^2 + |b|^2 + |c|^2 = 1$. The graph representation of the density matrix $|\psi\rangle_{123}^{W}\langle\psi|_{123}^{W}$ is given in the figure 2.9a. For a specific case, when $a = b = c = \frac{1}{\sqrt{3}}$, figure 2.9b represents a standard W state.

The four qubit cluster [Briegel and Raussendorf, 2001] and Chi [Yeo and Chua, 2006] states are given by $|\psi\rangle_{1234} = \frac{1}{2}(|0000\rangle + |0101\rangle + |1010\rangle - |1111\rangle)$ and $|\phi\rangle_{1234} = \frac{1}{2}(|0000\rangle + |0101\rangle + |1011\rangle - |1110\rangle)$, respectively. Their graph representations are depicted in the figure 2.10a and 2.10b.

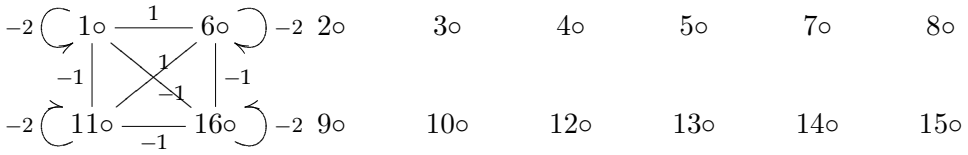
2.3.4 Werner state

A Werner state Werner [1989] is a bipartite mixed quantum state in $\mathcal{H}^{(d)} \otimes \mathcal{H}^{(d)}$. It is invariant under the unitary transformation $U \otimes U$, where U is an unitary operator acting on $\mathcal{H}^{(d)}$. It is represented by,

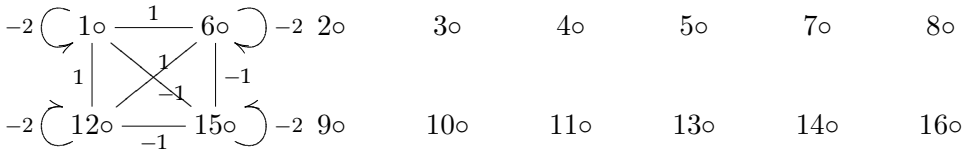
$$\rho_{x,d} = \frac{d-x}{d^3-d} I + \frac{xd-1}{d^3-d} F, \tag{2.26}$$

where $F = \sum_{i,j}^{d} |i\rangle\langle j| \otimes |j\rangle\langle i|$, $x \in [0,1]$ and d is the dimension of the individual subsystems. As the Werner state belongs to $\mathcal{H}^{(d)} \otimes \mathcal{H}^{(d)}$, the density matrix $\rho_{x,d}$ is a symmetric matrix of order d^2. All the Werner states are graph Laplacian states. As $\rho_{x,d}$ acts on the space $\mathcal{H}^{(d)} \otimes \mathcal{H}^{(d)}$, we partition the vertex set into d clusters $C_\mu, \mu = 1, 2, \ldots d$, each having d vertices. The corresponding digraph has three types of edges:

1. Loops at diagonal vertices $v_{11}, v_{22}, \ldots v_{dd}$ having loop weights $w(v_{\mu,\mu}, v_{\mu,\mu}) = (d-1)+(d-1)x$.
2. Loops at non-diagonal vertices $\{v_{\mu,i} : \mu \neq i\}$ having loop weights $w(v_{\mu,i}, v_{\mu,i}) = d - x$.
3. Non-loop edges with weight $w(v_{\mu,i}, v_{i,\mu}) = dx - 1$. Note that, there is only one edge between two different clusters. All such edges are diagonal and parallel to each-other.



(a) 4 qubit cluster states



(b) 4 qubit Chi state

Figure 2.10 : 4 qubit cluster and Chi states

The following example would help to illustrate this structure. Properties of Werner state will be discussed in the later chapters.

Example 2.5. *We may represent $\rho_{x,3}$, and $\rho_{x,4}$ as a graph with 9 and 16 vertices depicted in figure 2.11. The edge weights a, b, and c represents weights of different classes of edges discussed above.*

2.3.5 Isotropic state

An isotropic state belongs to $\mathcal{H}^{(d)} \otimes \mathcal{H}^{(d)}$. This state is invariant under the transformation $U \otimes U^\dagger$, where U is a unitary operator acting on $\mathcal{H}^{(d)}$. Its density matrix $\rho_{d,x}$ is defined by,

$$\rho_{d,x} = \frac{d^2}{d^2-1}\left[\frac{(1-F)}{d^2}I + \left(F - \frac{1}{d^2}\right)P\right], \tag{2.27}$$

where $F \in [0,1]$ is the fidelity of the quantum state and $P = |\psi\rangle\langle\psi|$ where $|\psi\rangle = \frac{1}{\sqrt{d}}\sum_i |i_a\rangle |i_b\rangle$, the maximally entangled state in dimension d. Considering diagonal and off-diagonal terms we may conclude that an isotropic quantum states is graphical provided

$$(d-1)\left|F - \frac{1}{d^2}\right| \leq \frac{d^2-1}{d^2}F. \tag{2.28}$$

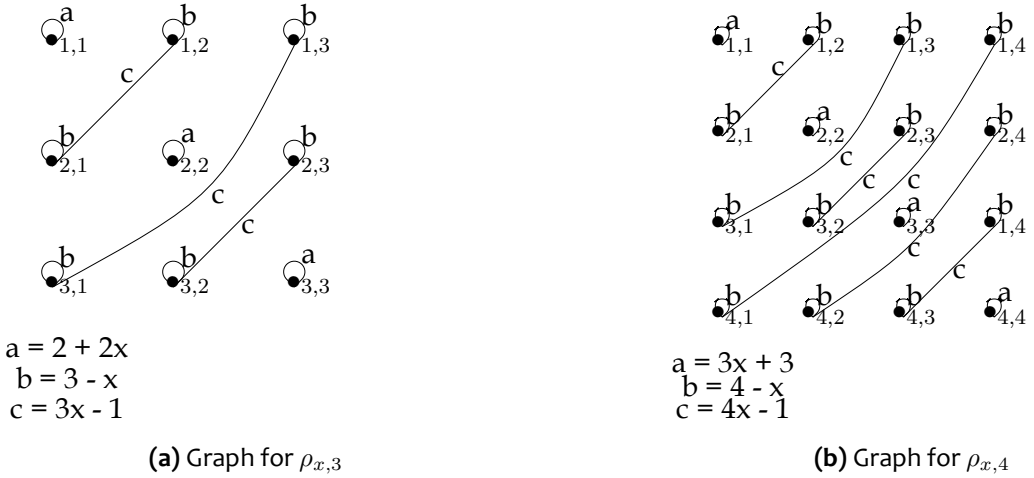
Putting $d = 2, 3, 4$ in the above equation we get, $\frac{1}{7} \leq F \leq 1$, $\frac{1}{13} \leq F \leq \frac{1}{5}$, $\frac{1}{11} \leq F \leq \frac{1}{21}$, respectively.

As $\rho_{d,x}$ acts on $\mathcal{H}^{(d)} \otimes \mathcal{H}^{(d)}$, we represent the vertex set into d clusters $C_\mu : \mu = 1, 2, \ldots d$ with $C_\mu = \{v_{\mu 1}, v_{\mu 2}, \ldots v_{\mu n}\}$. We observe that a graph representing an isotropic state has the following properties.

1. The diagonal vertices $v_{1,1}, v_{22}, \ldots v_{dd}$ form a complete graph which consists of all non-loop edges of the graph. Weight of these edges are $F - \frac{1}{d^2}$.

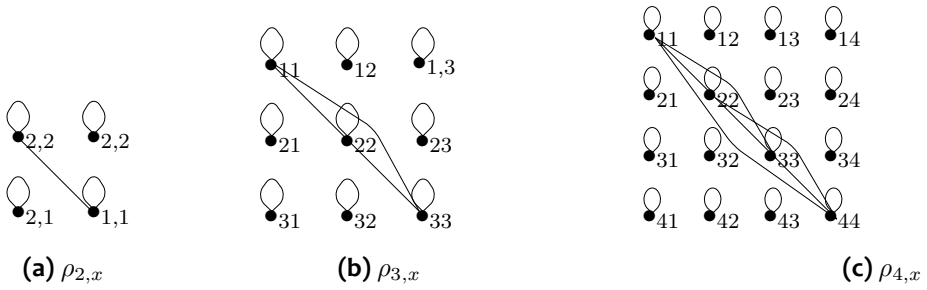
2. The loop weight of the non-diagonal vertices is $\frac{1-F}{d^2}$.

3. The loop weight of the diagonal vertices are given by $\frac{d^2-1}{d^2}F$.



(a) Graph for $\rho_{x,3}$ **(b)** Graph for $\rho_{x,4}$

Figure 2.11 : Graphs of some Werner states



(a) $\rho_{2,x}$ **(b)** $\rho_{3,x}$ **(c)** $\rho_{4,x}$

Figure 2.12 : Graphs of some Isotropic states.

All isotropic states are separable for $F < \frac{1}{d}$. Otherwise, they are entangled and violate the reduction criterion of separability.

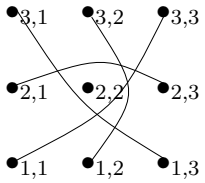
Example 2.6. *Graph representations of the isotropic state $\rho_{d,x}$ for $d = 2, 3, 4$ are depicted in the figure 2.12. In the picture, all the edges and loops are weighted as described above.*

2.3.6 X state

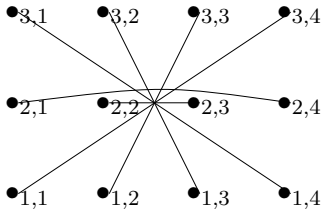
The X-state is well known in quantum information theory due to the specific structure of its density matrix. Here, we consider graph Laplacian X-states living in $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$. Hence, as before the vertex set of the corresponding digraph has m clusters $C_\mu, \mu = 1, 2, \ldots m$, each containing n vertices. The distribution of the non-zero elements in the density matrices suggests that the edge set has the following combinatorial characteristics:

1. If the bipartite subgraph $\langle C_\mu, C_\nu \rangle$ is non-empty then all the edges are of the form $(v_{\mu k}, v_{\nu(n-k)})$ for $k = 1, 2, \ldots n$.

2. There is only one non-empty subgraph $\langle C_\alpha \rangle$ with edges of the form $(v_{\alpha k}, v_{\alpha(n-k)})$ for $k = 1, 2, \ldots n$.



(a) X state acting on $\mathcal{H}^3 \otimes \mathcal{H}^3$.



(b) X state acting on $\mathcal{H}^3 \otimes \mathcal{H}^4$.

Figure 2.13 : Graphs of some X states.

Conversely, if the edge set of any graph follows the above two properties the corresponding quantum states will be classified as an X state.

Example 2.7. *Some of the graphs of X states without edge weights and directions are depicted in the figures 2.13a and 2.13b.*

2.4 WHAT NEXT?

We initiated this chapter with a minimal basic overview of quantum information theory. Then we have developed the idea of graph Laplacian states which was introduced in [Braunstein et al., 2006b]. Later it was extended for signless and signed Laplacian matrices of weighted digraphs in [Adhikari et al., 2017]. Investigating different properties of quantum states via combinatorial graphs is a broad general problem. We identify the following problems which have not been discussed earlier. They are important from the perspective of the interface of quantum information and graph theory, the subject of this thesis.

1. Unitary evolution of quantum states are well studied in quantum mechanics. In quantum information theory we use a number of unitary operators as the quantum counterpart of computational gates. Can we capture the action of quantum gates from a graph theoretic perspective?

2. Separability problem is interesting in quantum mechanics and information theory. How to detect an entangled state using its graph structure? An entangled state is generated from a separable state applying a global unitary transformation. Well know procedure of entanglement generation is the generation of Bell state. Can we generate a mixed entangled state from a mixed separable state? Note that, graph Laplacian states are mixed quantum states in general.

3. Quantum discord is another quantum correlation which has recently being used as a resource of quantum information. The reason behind classifying zero and non-zero quantum discord state is manifold. Can we classify the graph Laplacian states with zero discord?

4. The main theme of this work is in the interface of quantum information and graph theory. Are the techniques of quantum information theory useful for elucidation of non-trivial problems in graph theory?

The above questions will be discussed in the subsequent chapters of this thesis.