4

Graph Theoretic Aspects of Quantum Entanglement

In quantum mechanics, entanglement [Horodecki et al., 2009] is a feature implying the existence of a global state of a composite system which cannot be written as a product of individual subsystems. It may be regarded as the most non-classical manifestation of quantum mechanics [Neumann, 1932; Einstein et al., 1935]. The curious aspects of quantum entanglement has been debated upon for a long time in the course of the evolution of quantum mechanics. Progress has now been made to such an extent that entanglement is being utilized for practical aspects, such as in quantum teleportation [Bennett et al., 1993], cryptography [Bennett et al., 1992], and computation [Shor, 1995]. In this chapter, we shall study the detection of entangled Graph Laplacian quantum states [Dutta et al., 2016b].

4.1 AN INTRODUCTION TO QUANTUM ENTANGLEMENT

We begin this section with a simple example. Recall that, $|0\rangle = (1,0)^\dagger$. Consider the quantum state $|00\rangle = (1,0,0,0)^\dagger = (1,0)^\dagger \otimes (1,0)^\dagger = |0\rangle \otimes |0\rangle \in \mathcal{H}^{(2)} \otimes \mathcal{H}^{(2)}$. Clearly $|00\rangle$ can be written as a product of state vectors of the individual subsystems. We describe it as a product state. Similarly, $|11\rangle = |1\rangle \otimes |1\rangle$ is also a product state. But, their linear combination $|\phi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ cannot be written as $|\phi\rangle = |\phi\rangle_1 \otimes |\phi\rangle_2$ for $|\phi\rangle_1, |\phi\rangle_2 \in \mathcal{H}^2$. A state vector provides a complete description of a quantum system. Here, $|\phi\rangle$ provides a description of the system globally. As we can not write it as a product of state vectors of individual susbsystems we have no information about subsystems. We like to say $|\phi\rangle$ is an entangled state whereas $|00\rangle$ and $|11\rangle$ are separable states. Some other examples of entangled and separable two qubit states are as follows.

Example 4.1. *Consider α and $\beta \in \mathbb{C} - \{0\}$ such that $|\alpha|^2 + |\beta|^2 = 1$. Following states are separable two qubit states:*

$$\begin{aligned}
&|00\rangle = |0\rangle \otimes |0\rangle, && |11\rangle = |1\rangle \otimes |1\rangle, \\
&\alpha|00\rangle \pm \beta|01\rangle = |0\rangle \otimes (\alpha|0\rangle \pm \beta|1\rangle), && \alpha|10\rangle \pm \beta|11\rangle = |1\rangle \otimes (\alpha|0\rangle \pm \beta|1\rangle), \\
&\alpha|11\rangle \pm \beta|01\rangle = (\alpha|1\rangle \pm \beta|0\rangle) \otimes |1\rangle, && \alpha|10\rangle \pm \beta|00\rangle = (\alpha|1\rangle \pm \beta|0\rangle) \otimes |0\rangle.
\end{aligned} \tag{4.1}$$

Also $(\alpha|00\rangle \pm \beta|11\rangle)$, and $(\alpha|01\rangle \pm \beta|10\rangle)$ are two qubit entangled states.

Entanglement of Graph Laplacian states is our main concern in this chapter. Recall that a density matrix is a Hermitian, positive semi-definite, trace one matrix. Consider two density matrices $\rho_1 \in \mathcal{H}_1$ and $\rho_2 \in \mathcal{H}_2$. Clearly, $\rho_1 \otimes \rho_2$ is also a density matrix in $\mathcal{H}_1 \otimes \mathcal{H}_2$ and is a product state. A convex combination of these density matrices will also be a density matrix. We call it a separable state. Mathematically, we may define separability and entanglement as follows:

Definition 4.1. Separability and entanglement *A quantum state $|\psi\rangle$ is separable if*

$$|\psi\rangle = \sum \alpha_i |\psi\rangle_i^{(A)} \otimes |\psi\rangle_i^{(B)}, \text{ where } \sum_i |\alpha_i| = 1.$$

In terms of density matrix, a quantum state represented by $\rho(G)$ is separable if

$$\rho = \sum p_i \rho_i^{(A)} \otimes \rho_i^{(B)}, \text{ where } p_i > 0 \text{ and } \sum_i p_i = 1.$$

Otherwise, the state is entangled.

We have already mentioned that entanglement is used as a resource in quantum information and computation. Hence, detecting entanglement is crucial. Familiar methods in this context are Peres-Horodecki criterion [Peres, 1996; Horodecki, 1997], entanglement witness [Horodecki et al., 2001; Terhal, 2000], matrix realignment criterion [Rudolph, 2003; Chen and Wu, 2002], reduction criterion [Cerf et al., 1997; Horodecki and Horodecki, 1999]. Some reviews on entanglement include [Terhal, 2002; Horodecki et al., 2009; Krammer, 2005].

In general a density matrix $\rho \in \mathcal{H}_A \otimes \mathcal{H}_B$ can be expressed as,

$$\rho = \sum_{ijkl} p_{kl}^{ij} \left|i\right\rangle \left\langle j\right| \otimes \left|k\right\rangle \left\langle l\right|. \tag{4.2}$$

The partial transpose with respect to the second subsystem is given by,

$$\rho^{T_B} = \sum_{ijkl} p_{kl}^{ij} \left|i\right\rangle \left\langle j\right| \otimes (\left|k\right\rangle \left\langle l\right|)^t = \sum_{ijkl} p_{lk}^{ij} \left|i\right\rangle \left\langle j\right| \otimes \left|l\right\rangle \left\langle k\right|. \tag{4.3}$$

Let ρ be a separable state. Then using definition 4.1 it can be written as,

$$\rho = \sum p_i \rho_i^{(A)} \otimes \rho_i^{(B)}. \tag{4.4}$$

Now the partial transpose is

$$\rho^{T_B} = \sum p_i \rho_i^{(A)} \otimes (\rho_i^{(B)})^t. \tag{4.5}$$

The operation of conjugate transpose does not alter the eigenvalues. As $\rho_i^{(B)}$ is a density matrix, $(\rho_i^{(B)})^\dagger$ will also be a density matrix. Ultimately, if ρ is separable ρ^{T_B} will also be a positive semi-definite matrix. This may be expressed as,

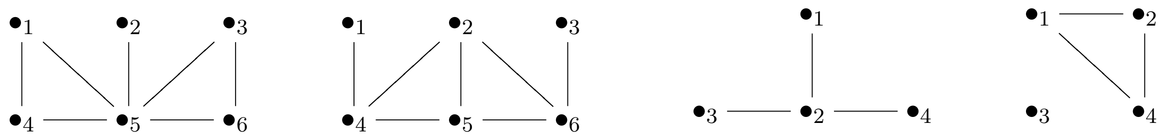
Definition 4.2. Positive partial transpose (PPT) criterion: *If the density matrix ρ represents a separable state in $\mathcal{H}_A \otimes \mathcal{H}_B$ then ρ^{T_B} is a positive semi-definite matrix.*

Clearly, PPT criterion is a necessary condition for separability. It is sufficient for states in $\mathcal{H}^{(2)} \otimes \mathcal{H}^{(2)}$ [Peres, 1996], $\mathcal{H}^{(2)} \otimes \mathcal{H}^{(3)}$ [Horodecki, 1997], and for low rank density matrices [Horodecki et al., 2000]. In higher dimension, it is also sufficient under some given conditions.

4.2 GRAPH THEORETIC ASPECTS OF PARTIAL TRANSPOSE

Partial transpose, which is used in quantum information theory, due to a deep significance in operator theory, has a graph theoretical analogue. In this section, we discuss its graph theoretic counterpart. We apply it for obtaining separability criterion of graph Laplacian quantum states, in the next section [Dutta et al., 2016b]. The graph theoretic partial transpose was first developed in [Wu, 2006b].

In chapter 2, we have constructed a relation between clustering on vertex set and the blocks of a density matrix. The clustering on the vertex set was given in equation (2.14). For simplicity we may say that partial transpose on the second subsystem is the transpose on the blocks of the density matrix. Transpose on the blocks can be expressed as an operation on the edges joining vertices of two layers as follows:



(a) A pair of cospectral graphs

(b) A pair of signless Laplacian cospectral graphs

Figure 4.1 : GTPT equivalent non-isomorphic graphs

Definition 4.3. GTPT: *Given a clustered graph G with $m \times n$ vertices and clusters $C_\mu = \{v_{\mu,1}, v_{\mu,2}, \dots v_{\mu,n}\}$ for $\mu = 1, 2, \dots m$, the Graph Theoretical Partial Transpose (GTPT) involves replacing all existing edges $(v_{\alpha,i}, v_{\beta,j})$, with $\alpha \neq \beta$, and $i \neq j$ with the non-existing edges $(v_{\alpha,j}, v_{\beta,i})$.*

It is clear form this definition that GTPT generates a clustered graph $G^\tau = (V(G), E(G^\tau))$ from a graph $G = (V(G), E(G))$. We call G and G^τ as GTPT equivalent. Note that, the number of vertices and edges in G and G^τ are equal. Now we investigate some relations between them. The following lemma is trivial as replacement of edges $(v_{\mu,i}, v_{\nu,j}), \mu \neq \nu, i \neq j$ by $(v_{\mu,j}, v_{\nu,i})$ introduce transpose in the blocks of $A(G)$.

Lemma 4.1. *Given a clustered graph G, with $m \times n$ vertices and clusters $C_\mu = \{v_{\mu,1}, v_{\mu,2}, \dots v_{\mu,n}\}$ for $\mu = 1, 2, \dots m$, we have $A(G^\tau) = A(G)^{T_B}$, where $A(G)$ and $A(G^\tau)$ are adjacency matrices of the graph G and G^τ.*

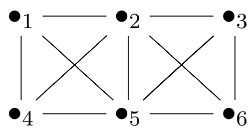
Depending on graph G, the degree sequences of G and G^τ can be different. There is at least one $i \in V(G)$ s.t. degree of i in G, $d_G(i) \neq d_{G^\tau}(i)$. Hence, degree matrices are also different, $D(G^\tau) \neq D(G)$. But as $D(G)$ is a diagonal matrix, $D(G)^{T_B} = D(G) \Rightarrow D(G)^{T_B} \neq D(G^\tau)$. Finding properties of GTPT equivalent graphs are important as partial transpose is a significant tool in entanglement detection. Two GTPT equivalent graphs G and G^τ may not be isomorphic and hence may not have equal spectra. Below we provide some examples of interest to graph theory. We will come back to this, in Chapter 6.

Example 4.2. *Graphs shown in figure 4.1a are non-isomorphic but their adjacency matrices have equal spectra. Also, consider the graph G and G^τ in figure 4.1b. Here G and G^τ are non-isomorphic but their signless Laplacian matrices have equal spectra.*

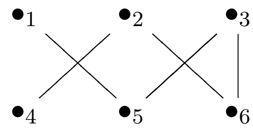
In the present context we are interested in those graphs which remains invariant under partial transpose and call them partially symmetric graphs. Idea of partial symmetry is different from the conventional idea of symmetry in graphs.

Definition 4.4. Partial Symmetry: *A clustered graph G of $m \times n$ vertices with clusters $C_\mu = \{v_{\mu,1}, v_{\mu,2}, \dots v_{\mu,n}\}$ for $\mu = 1, 2, \dots m$ is a partially symmetric if $(v_{\mu,i}, v_{\nu,j}) \in E(G)$ indicates $(v_{\mu,j}, v_{\nu,i}) \in E(G)$ for all μ, ν, i, j and $\mu \neq \nu$.*

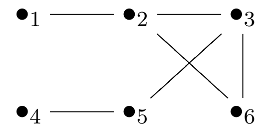
Therefore, a graph G is partially symmetric if all its subgraphs $\langle C_\mu, C_\nu \rangle$ are partially symmetric. Note that, if $\langle C_\mu, C_\nu \rangle$ is an empty graph then it is trivially partially symmetric. We call the edges $(v_{\mu,i}, v_{\nu,j}) \in E(G)$ and $(v_{\mu,j}, v_{\nu,i}) \in E(G)$ complement to each other. When a graph is partial symmetric with respect to some vertex labelling, every edge joining two vertices belonging to the two layers has its complement. The following properties of partially symmetric graph G are immediate.



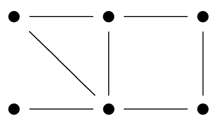
(a) Complete graph of order 6



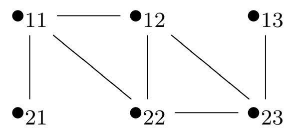
(b) Partially symmetric path graph



(c) Asymmetric graph which is partially symmetric.



(d) Asymmetric graph which is not partially symmetric



(e) A symmetric graph which is not partially symmetric

Figure 4.2 : Example and non-examples of partially symmetric graphs

1. A partial symmetric graph may not be connected.
2. Chromatics number of $G \leq \min\{m, n\}$.
3. Obviously $A(G) = A(G^\tau)$.
4. Given a partial symmetric graph $D(G) = D(G^\tau)$.
5. Two GTPT equivalents graphs G and G^τ are isomorphic.

Partial symmetry is not a structural property of a graph. Depending on vertex labellings two isomorphic graphs may not be partially symmetric. In the next example we mentions some graphs which are partially symmetric with respect to at least one vertex labellings.

Example 4.3. *A complete graph (figure 4.2a) of composite order with clusters is always a partially symmetric graph with respect to any vertex labelling. A complete multi-partite graph with equal partitions and usual vertex labellings is a partially symmetric graph. For every path of even order there is a vertex labelling such that it is partially symmetric. Consider the figure 4.2b. Similarly, an even cycle is partially symmetric. Tensor product of two graphs are partially symmetric. The idea of partial symmetry is different from the conventional idea of symmetry in graph theory. Given an asymmetric graph there may be a vertex labeling such that it is a partially symmetric graph. Consider the graph in the figure 4.2c. Also there are asymmetric graphs which are not partially symmetric with respect to any vertex labelling. One such example is shown in figure 4.2d. A symmetric graph may be partially symmetric. Consider the graph in figure 4.2e.*

4.3 SEPARABILITY CONDITION ON GRAPHS

We begin this section recalling the definition 4.1 of separability. A bipartite quantum state represented by a density matrix ρ is is separable if $\rho = \sum_i p_i \rho_i^{(A)} \otimes \rho_i^{(B)}$ where $p_i > 0$ and $\sum_i p_i = 1$. Otherwise, ρ is entangled. We have also mentioned that PPT criterion is a necessary condition of separability. But in higher dimensions there are entangled states which satisfies PPT criterion. We call them bound entangled states [Bennett et al., 1999]. There are graph Laplacian bound entangled states also. Proving separability of a given class of entangled states is a formidable task. But, imposing additional conditions with PPT criterion generates classes of new separable states. In this section, we collect some of these classes of graph Laplacian quantum states. Recall that, we have considered two density matrices $\rho_l(G)$ and $\rho_q(G)$ corresponding to the Laplacian and the signless Laplacian matrix of the graph G.

Theorem 4.1. *The density matrices $\rho(G)$ and $\rho(G^\tau)$ are separable together if $D(G) = D(G^\tau)$.*

Proof. Let $\rho(G) = \rho_l(G)$. Consider $\rho_l(G)$ is separable. Thus $\rho_l(G) = \sum_i p_i \rho_i^A \otimes \rho_i^B$. Therefore,

$$\begin{aligned}
\rho_l(G)^{T_B} &= \sum_i p_i \rho_i^A \otimes (\rho_i^B)^{T_B} \\
&= \frac{1}{\text{trace}(L(G))}(L(G))^{T_B} = \frac{1}{\text{trace}(L(G))}((D(G))^{T_B} - (A(G))^{T_B}) \\
&= \frac{1}{\text{trace}(L(G))}(D(G) - A(G^\tau)) \\
&= \frac{1}{\text{trace}(L(G))}(D(G) - D(G^\tau) + D(G^\tau) - A(G^\tau)) \\
&= \frac{1}{\text{trace}(L(G))}(D(G) - D(G^\tau) + L(G^\tau)) \\
&= \frac{1}{\text{trace}(L(G^\tau))}L(G^\tau) + \frac{1}{\text{trace}(L(G))}(D(G) - D(G^\tau)) \\
&\quad [\because d(G) = d(G^\tau) \Rightarrow \text{trace}(L(G)) = \text{trace}(L(G^\tau)).] \\
\rho_l(G^\tau) &= \rho_l(G)^{T_B} - \frac{1}{\text{trace}(L(G))}(D(G) - D(G^\tau)) \\
&= \sum_i p_i \rho_i^A \otimes (\rho_i^B)^{T_B} - \frac{1}{\text{trace}(L(G))}(D(G) - D(G^\tau)) \\
\rho_l(G^\tau)^{T_B} &= \sum_i p_i \rho_i^A \otimes \rho_i^B - \frac{1}{\text{trace}(L(G))}(D(G) - D(G^\tau)) \ [\because (D(G))^{T_B} = D(G).]
\end{aligned} \tag{4.6}$$

Thus, $\rho_l(G^\tau)$ is separable, when $D(G) = D(G^\tau)$.

Now we assume that $\rho(G) = \rho_q(G)$ and $\rho_q(G)$ is separable. In a similar fashion, $\rho_q(G^\tau)^{T_B} = \sum_i p_i \rho_i^A \otimes \rho_i^B + \frac{1}{\text{trace}(Q(G))}(D(G) - D(G^\tau))$, assuming, $\rho_q(G^\tau) = \sum_i p_i \rho_i^A \otimes \rho_i^B$. Thus, $\rho_q(G^\tau)$ is separable, when $D(G) = D(G^\tau)$. □

This theorem has a number of implications. We have a pair of graphs G and G^τ with equal degree matrices. If we know $\rho(G)$ is separable, then immediately $\rho(G^\tau)$ is also separable. Suppose G and G^τ are non-isomorphic having same degree sequence. Now by the above theorem, both of them are separable. Therefore, in this case separability does not help in solving graph isomorphism problem.

In the previous section, we have seen that partial symmetry keeps the graph unchanged under partial transpose. Thus density matrices corresponding to the partially symmetric graphs remains positive semi-definite after partial transpose which is a necessary condition of separability. Imposing additional criterion ensures separability. Also, partial symmetry keeps the density matrix unchanged. This provides another motivation to investigate separability property of $\rho(G)$ for partially symmetric graphs.

Theorem 4.2. *If the following criterion are satisfied by a partially symmetric graph G then $\rho(G)$ is separable:*

1. *Between two vertices belonging to a layer C_μ, there is no edge for all μ.*

2. *Degree of all the vertices of a partition is equal, that is, $d(v_r) = d(v_s)$ for all $v_r, v_s \in C_\mu$ and for all μ.*

3. *Either the subgraph $\langle C_\mu, C_\nu \rangle$ is empty or any two non-empty induced subgraphs $\langle C_\alpha, C_\beta \rangle$ and $\langle C_\mu, C_\nu \rangle$ are equal.*

Proof. As there is no edge joining two vertices of a layer C_μ, $A_{\mu,\mu} = 0$ for all μ. Also, vertices of same partition have equal degree. Therefore, the degree submatrix of the $D_\mu = \text{diag}\{d_\mu\} = d_i.I$.

As pattern of edge distribution between different modules are same, $A_{\alpha,\beta} = A_{\mu,\nu}$, for all α, β, μ, ν; if there is no edge joining C_μ and C_ν, $A_{\mu,\nu} = 0$. Also, $A_{\mu,\nu}$ is a symmetric matrix because G is partially symmetric graph. Therefore for $A_{\mu,\nu} \neq 0$ we can write

$$A_{\mu,\nu} = \sum_r \lambda_r u_r u_r^\dagger, \tag{4.7}$$

where u_r is a normalised eigenvector that is $u_r u_r^\dagger$ is trace 1 positive semi-definite matrix. Also $A_{\mu,\nu} = A_{\nu,\mu} = A_{\mu,\nu}^\dagger$. If $A_{\mu,\nu} = 0$ we can write $A_{\mu,\nu} = \sum_r 0.u_r u_r^\dagger$. The proof does not differ much for $A_{\mu,\nu} = 0$. Therefore, we assume that $A_{\mu,\nu} \neq 0$ for all μ, ν. Now,

$$\begin{aligned}
L(G) &= \begin{bmatrix} d_1.I & A_{1,2} & A_{1,3} & \dots & A_{1,m} \\ A_{2,1} & d_2.I & A_{2,3} & \dots & A_{2,m} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{m,1} & A_{m,2} & A_{m,3} & \dots & d_m.I \end{bmatrix} \\
&= \begin{bmatrix} d_0 \sum_r u_r u_r^\dagger & \sum_r \lambda_r u_r u_r^\dagger & \sum_r \lambda_r u_r u_r^\dagger & \dots & \sum_r \lambda_r u_r u_r^\dagger \\ \sum_r \lambda_r u_r u_r^\dagger & d_1 \sum_r u_r u_r^\dagger & \sum_r \lambda_r u_r u_r^\dagger & \dots & \sum_r \lambda_r u_r u_r^\dagger \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_r \lambda_r u_r u_r^\dagger & \sum_r \lambda_r u_r u_r^\dagger & \sum_r \lambda_r u_r u_r^\dagger & \dots & d_{(m-1)} \sum_r u_r u_r^\dagger \end{bmatrix} \\
&= \sum_r \begin{bmatrix} d_1 & \lambda_r & \lambda_r & \dots & \lambda_r \\ \lambda_r & d_2 & \lambda_r & \dots & \lambda_r \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \lambda_r & \lambda_r & \lambda_r & \dots & d_m \end{bmatrix} \otimes u_r u_r^\dagger = \sum_r B \otimes u_r u_r^\dagger,
\end{aligned} \tag{4.8}$$

where $B = \begin{bmatrix} d_1 & \lambda_r & \lambda_r & \dots & \lambda_r \\ \lambda_r & d_2 & \lambda_r & \dots & \lambda_r \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \lambda_r & \lambda_r & \lambda_r & \dots & d_m \end{bmatrix}$. Note that, $A_{i,j} = 0 \Rightarrow b_{i,j} = 0$. We claim that B is a positive semi-definite matrix, which will be proved later. We have degree of the graph $d(G) = \sum_\mu d_\mu = \text{trace}(B)$. Therefore, $\frac{B}{\text{trace } B} = \frac{B}{d(G)}$ is a matrix of unit trace. Now,

$$\rho_l(G) = \frac{1}{d(G)} L(G) = \sum_r \frac{B}{d(G)} \otimes u_r u_r^\dagger. \tag{4.9}$$

Hence, $\rho_l(G)$ is separable. In a similar fashion, we can show that $\rho_q(G)$ is also separable.

Now we have to prove our claim that B in the above equation is a positive semi-definite matrix. First we recall the definition 2.13 of a diagonally dominant matrix. Let us assume, $A_{\mu,\nu} = (a_{ij})_{n \times n}$. Note that, the spectral radius of $A_{\mu,\nu} \leq ||A_{\mu,\nu}||_\infty$, where $||A_{\mu,\nu}||_\infty$ is the subordinate

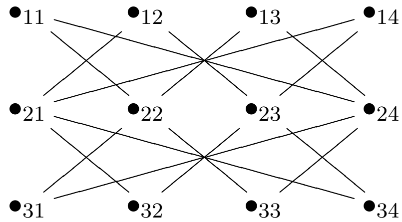


Figure 4.3 : Example of theorem 4.2.

matrix norm defined by $||A_{\mu,\nu}||_\infty = \max_i \sum_{j=1}^{n} |a_{i,j}|$. Additionally,

$$d_i = \sum_{k=0}^{m-1} \max_i \sum_{j=1}^{n} |a_{i,j}| = m \max_i \sum_{j=1}^{n} |a_{i,j}|. \tag{4.10}$$

Therefore, $(m-1)\lambda_r \leq (m-1) \times ($ Spectral radius of $A_{\mu,\nu}) \leq d_\mu$ for all μ. Hence, B is a diagonally dominant, Hermitian matrix. Its diagonal entries are positive real numbers. Therefore B is a positive semi-definite matrix. $\square$

The following graph satisfies all the conditions satisfying the above theorem. Thus, quantum states represented by its density matrices are separable.

Example 4.4. *Consider the graph G in figure 4.3. It has three clusters C_1, C_2 and C_3 each containing four vertices. Between two vertices of a layer there is no edge. In a layer degree of vertices is two. The subgraph $\langle C_1, C_3\rangle$ is empty. Also two non-empty induced subgraphs $\langle C_1, C_2\rangle$ and $\langle C_2, C_3\rangle$ are equal. Therefore, G satisfies all the conditions of the theorem 4.2. Thus, $\rho(G)$ is separable.*

In theorem 4.2 we did not consider an edge between two vertices of a cluster. But in the next lemma we have assumed those edges to generate a class of separable states. Before that we present a standard definition of graph theory.

Definition 4.5. Union of graphs: *The union graph of two graphs $G = (V(G), E(G))$ and $H = (V(H), E(H))$ is defined by a new graph $G \cup H = (V(G) \cup V(H), E(G) \cup E(H))$.*

Let G be a graph of order n with vertex labelling $\{v_1, v_2, \dots v_n\}$. The union of m copies of G is given by a graph, $mG = G \cup G \cup \dots \cup G$ with vertex labelling $\{v_{\mu,i} : \mu = 1, 2, \dots m$ and $i = 1, 2, \dots n\}$. Therefore, copies of G construct the layers of mG. Note that, there is no edge between two vertices belonging to two different clusters. Hence, mG is trivially partially symmetric and it violates the 1-st condition of Theorem 4.2. Interestingly, we will show now that mG represents separable states.

Lemma 4.2. *Given a graph G, the density matrix $\rho(mG)$ represent a bipartite separable state with respect to the standard vertex labelling on mG.*

Proof. We observe that

$$\begin{aligned}
A(mG) &= \text{diag}\{A(G), A(G), \dots, A(G)(m \text{ times})\} &= I_m \otimes A(G),\\
D(mG) &= \text{diag}\{D(G), D(G), \dots, D(G)(m \text{ times})\} &= I_m \otimes D(G),\\
L(mG) &= \text{diag}\{L(G), L(G), \dots, L(G)(m \text{ times})\} &= I_m \otimes L(G),\\
Q(mG) &= \text{diag}\{Q(G), Q(G), \dots, Q(G)(m \text{ times})\} &= I_m \otimes Q(G).
\end{aligned} \tag{4.11}$$

where, I_m denotes the identity matrix of order m. Now I_m is a positive semi-definite Hermitian matrix. Thus, $\rho_l(mG) = \frac{L(mG)}{\text{trace}(L(mG))}$ and $\rho_q(mG) = \frac{Q(mG)}{\text{trace}(Q(mG))}$ are separable states. □

Now we are in position to generalize the theorem 4.2 using the last lemma. Let G be a graph with n vertices and H be a partially symmetric graph satisfying all the conditions of result 4.2 with m different clusters. We construct a new graph $G \bowtie H$ by placing m copies of G on m clusters of H. It is easy to show that $\rho(G \bowtie H)$ is a separable state.

Lemma 4.3. *$L(G \bowtie H) = L(H) + L(mG)$. Also. $Q(G \bowtie H) = Q(G) + Q(H)$.*

Proof. The graph mG is an union of m copies of G. Thus, $A(mG) = \text{diag}\{A(G), A(G), \dots A(G)\}$. As H satisfies the conditions of theorem 4.2 there is no edge between two vertices belonging to same clusters. Thus the diagonal blocks of H are zero matrices. After putting m copies of G in the clusters of H the diagonal bolcks of $G \bowtie H$ are $A(G)$. Therefore, it is clear from the construction of $G \bowtie H$ that $A(G \bowtie H) = A(H) + A(mG)$. Now considering the Laplacian and the signless Laplacian matrices we get the result. □

Theorem 4.3. *The quantum state represented by the density matrix $\rho(G \bowtie H)$ is a separable state in $\mathcal{H}^{(n)} \otimes \mathcal{H}^{(m)}$.*

Proof. Dividing the Laplacian and signless Laplacian matrices of $G \bowtie H$ by their traces we get $\rho(G \bowtie H) = \rho(mG) + \rho(H)$. We have proved that $\rho(H)$ and $\rho(mG)$ are separable states. We know that a convex combination of separable states is separable. Thus, $\rho(G \bowtie H)$ is also separable. □

Our results provide methods for constructing classes of new separable states in higher dimensions. Here we present an example in support of theorem 4.3.

Example 4.5. *Consider the graphs G and H in the figure 4.4a and 4.4b. Note that, graph H satisfies all the conditions of theorem 4.2. The graph $G \bowtie H$ is shown in the figure 4.4c. Applying the theorem 4.3 we say the density matrix $\rho(G \bowtie H)$ is separable.*

We end the section with an example of Graph Laplacian entangled quantum state state represented by a graph which is not partially symmetric.

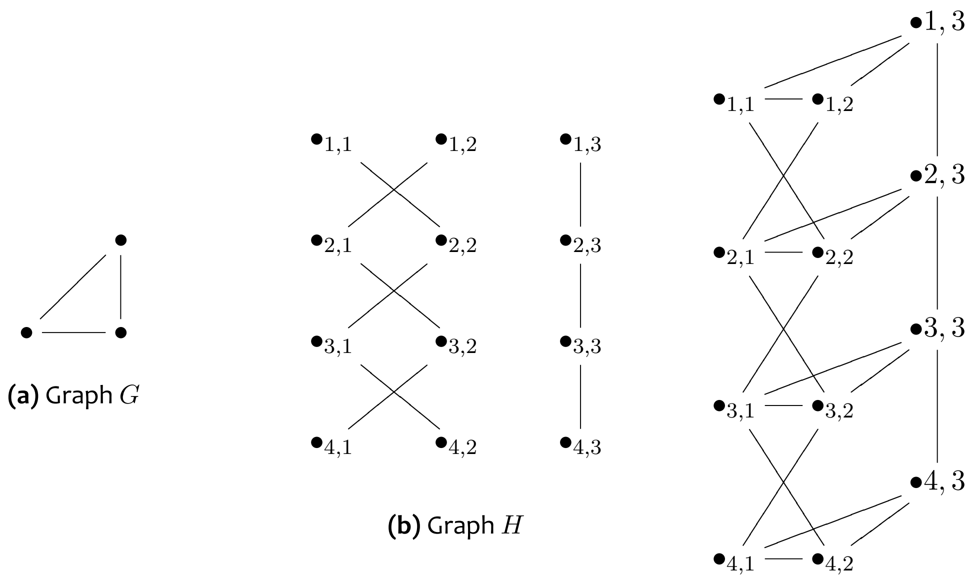
Example 4.6. *Werner state is a mixture of projectors onto the symmetric and antisymmetric subspaces, with the relative weight p_{sym} being the only parameter that defines the state.*

$$\rho(d, p_{sym}) = p_{sym} \frac{2}{d^2 + d} P_{sym} + (1 - p_{sym}) \frac{2}{d^2 - d} P_{as}, \tag{4.12}$$

where, $P_{sym} = \frac{1}{2}(1+P), P_{as} = \frac{1}{2}(1-P)$, are the projectors and $P = \sum_{ij} |i\rangle \langle j| \otimes |j\rangle \langle i|$ is the permutation operator that exchanges the two subsystems.

The quantum state $\rho(d, 0) = \frac{I-P}{d^2-d}$ is represented by Laplacian matrix of simple graphs. We know that $\rho(d, 0)$ is an entangled state. The density matrix $\rho(2, 0)$ is given by,

$$\rho(2, 0) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & .5 & -.5 & 0 \\ 0 & -.5 & .5 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} = \rho_l(G), \tag{4.13}$$



(a) Graph G

(b) Graph H

(c) Graph $G \bowtie H$

Figure 4.4 : Example of theorem 4.3.

for the graph G depicted in figure 4.5a. Also, the state $\rho(3,0)$ *is represented by the graph in the figure 4.5b, where*

$$\rho(3,0) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.1667 & 0 & -0.1667 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.1667 & 0 & 0 & 0 & -0.1667 & 0 & 0 \\ 0 & -0.1667 & 0 & 0.1667 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.1667 & 0 & -0.1667 & 0 \\ 0 & 0 & -0.1667 & 0 & 0 & 0 & 0.1667 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.1667 & 0 & 0.1667 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{4.14}$$

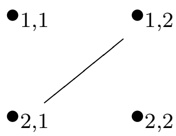
Note that, none of these graphs are partially symmetric. Any subgraph $\langle C_\mu, C_\nu \rangle$ *consists of exactly one edge of the form* $(v_{\mu,\nu}, v_{\nu,\mu})$*. But the edge* $(v_{\mu,\mu}, v_{\nu,\nu})$ *is absent.*

4.4 GRAPH ISOMORPHISM AND QUANTUM ENTANGLEMENT

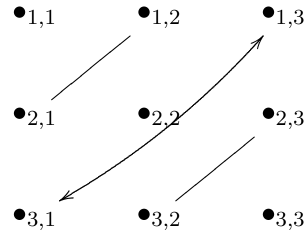
In chapter 3, we have studied CNOT gate operation on graphs. Recall that,

$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{4.15}$$

A permutation matrix P contains a 1 in every row and column, remaining all elements are zero. Therefore, $CNOT$ is a permutation matrix. Now recall the definition 2.3 of graph isomorphism



(a) Graph of $\rho(2,0)$.



(b) Graph of $\rho(3,0)$.

Figure 4.5 : Graphs for entangled Werner states

discussed in Chapter 2. If two graphs G and H are isomorphic then there is a permutation matrix P such that $\rho(H) = P\rho(G)P^{\dagger}$. If $\rho(G)$ is entangled in $\mathcal{H}^{(p)} \otimes \mathcal{H}^{(q)}$, $\rho(H)$ need not be entangled in $\mathcal{H}^{(p)} \otimes \mathcal{H}^{(q)}$. There are a number of graphs for which the separability property does not depend on graph isomorphism. We mention two results form [Braunstein et al., 2006b].

Theorem 4.4. *For any $N = n \times m$ the density matrix $\rho(K_N)$ represents a separable state in $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$, where K_N denotes a complete graph of order N.*

Theorem 4.5. *For any $N = n \times m \geq 4$, the density matrix of a star graph $\rho(K_{1,N-1})$ is entangled in $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$.*

Note that, in the above two results separability does not depend on the graph isomorphism or the vertex labellings on them. But consider the following example,

Example 4.7. *Here, we consider two isomorphic copies of a path graph depicted in the figure 4.6. Considering the vertex labellings in the figure 4.6b we find the density matrix,*

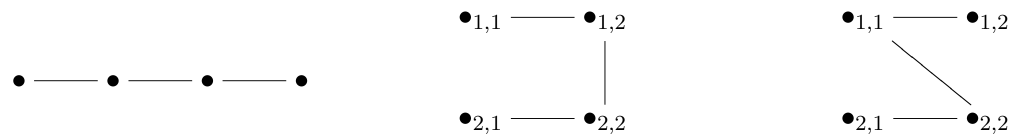
$$\rho(G) = \frac{1}{6}\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 2 & 0 & 1 \\ 1 & 0 & 2 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}. \tag{4.16}$$

We also consider the density matrix of the path graph with respect to the vertex labellings depicted in 4.6c which is

$$\rho(H) = \frac{1}{6}\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}. \tag{4.17}$$

Clearly, $\rho(G)$ and $\rho(H)$ represents two qubit density matrices. A simple calculation using PPT criterion shows that $\rho(G)$ is separable but $\rho(H)$ is entangled. The graph isomorphism acting here is given by $u : G_1 \to G_2$ where, $u(1) = 2, u(2) = 1, u(3) = 3, u(4) = 4$. Also, the permutation matrix corresponding to this permutation is,

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{4.18}$$



(a) A path graph **(b)** Separable **(c)** Entangled

Figure 4.6 : Two isomorphic copies of a path graph with different separability properties

Therefore, we may classify all the graphs into three classes as follows:

1. **S-Graphs :** All the vertex labelling on G generates separable states. For example, consider complete graphs.
2. **E-Graphs:** All the vertex combination on G generates entangled states. For example, consider the star graphs.
3. **SE-Graphs:** Here different vertex labellings produce both entangled and separable states. For example consider the path graph.

Therefore, graph isomorphism has a specific significance for SE graphs as they can convert a mixed separable state to a mixed entangled state. In this way, graph isomorphism acts as an entanglement generator for Graph Laplacian quantum states. Note that, the PPT criterion is necessary and sufficient for quantum states in $\mathcal{H}^{(2)} \otimes \mathcal{H}^{(2)}$ and $\mathcal{H}^{(2)} \otimes \mathcal{H}^{(3)}$. Therefore, all quantum states represented by a partial symmetric graph of order ≤ 6 is separable. Consider the following example:

Example 4.8. *Consider two isomorphic graphs in the figure 4.7. Graph G in the figure 4.7a is separable state. Note that, it is partially symmetric and its order is ≤ 6. An isomorphic copy H of G is depicted in 4.7b, which is entangled. The corresponding permutation is given by*

$$\begin{pmatrix} 11 & 12 & 13 & 21 & 22 & 23 \\ 13 & 11 & 23 & 21 & 22 & 12 \end{pmatrix}. \tag{4.19}$$

The permutation matrix is

$$P = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{4.20}$$

Note that, the matrix P different from $CNOT$. Also $\rho(H) = P\rho(G)P^{\dagger}$.

4.5 WHAT NEXT?

The crucial philosophy behind this work is that graph isomorphism can be utilized in generating mixed entangled states from graph Laplacian separable states. We have also established a number of sufficiency conditions of separability in higher dimensions. This opens up a number of problems for future consideration, such as:

(a) Mixed separable state

(b) Mixed entangled state

Figure 4.7 : Mixed separable state to mixed entangled state via graph isomorphism.

1. Though we have generated some classes of separable bipartite states in higher dimensions, we need other classes of such states to get a more complete picture of bipartite separability. We have seen that partial symmetric graphs provide separable states under some additional condition. Yet the scenario is not transparent for other partial symmetric graphs. Bound entangled states fulfil PPT criterion. Is there any partially symmetric graph Laplacian bound entangled state? What are the graphical criterion to be a bound entangled state?

2. Graph isomorphism can be used as an entanglement generator for ES-Graphs. Different isomorphic copies of an ES-Graph have different separability properties. Thus we need to find graphical conditions for a graph to be an ES-Graph.

3. Another immediate generalization of this work can be done for multipartite systems. Multipartite entanglement is useful in quantum information theory. But characteristics of graph Laplacian multipartite entangled states are not well studied. Very recently a work has come in this direction [Zhao et al., 2017].

4. We have seen that there are GTPT equivalent cospectral, non-isomorphic graphs. In graph theory finding classes of non-isomorphic, cospectral graphs is an important problem. We shall have further discussions in this direction in Chapter 6.