# Bipartite separability and non-local quantum operations on graphs

Supriyo Dutta
*Department of Mathematics, Indian Institute of Technology Jodhpur, Jodhpur 342011, India**

Bibhas Adhikari
*Department of Mathematics, Indian Institute of Technology Kharagpur, Kharagpur 721302, India*†

Subhashish Banerjee
*Department of Physics Indian Institute of Technology Jodhpur, Jodhpur 342011, India*‡

R. Srikanth
*Poornaprajna Institute of Scientific Research, Bangalore, Karnataka 560080, India*§

**Abstract** In this paper, we consider the separability problem for bipartite quantum states arising from graphs. Earlier it was proved that the degree criterion is the graph theoretical counterpart of the familiar PPT criterion for separability, although there are entangled states with positive partial transpose for which degree criterion fails. Here, we introduce the concept of partially symmetric graphs and degree symmetric graphs by using the well-known concept of partial transposition of a graph and degree criteria, respectively. Thus, we provide classes of bipartite separable states of dimension $m \times n$ arising from partially symmetric graphs. We identify partially asymmetric graphs which lack the property of partial symmetry. Finally we develop a combinatorial procedure to create a partially asymmetric graph from a given partially symmetric graph. We show that this combinatorial operation can act as an entanglement generator for mixed states arising from partially symmetric graphs.

## I. INTRODUCTION

Graph theory [1, 2] is a well-established branch of mathematics. It forms the core of complex systems [3, 4], widely used in Economics, Social Science and System Biology [5], as well as in communication and information [6]. It is also used to address foundational aspects of different branches of mathematics and physics [7]. To the best of our knowledge, combinatorial graphs have been used in quantum mechanics and information theory [8] in four different ways: (a). **Quantum Graphs:** Here, a differential or pseudo-differential operator is associated with a graph. The operator acts on functions defined on each edge of the graph when the edges are equipped with compact real intervals. [9, 10]. (b). **Graph states:** In this approach, combinatorial graphs are used to describe interactions between different quantum states [11–13]. Here the vertices of the graph represent the quantum mechanical states, while the interactions between them are represented by the edges. Graph states were proposed as a generalization of cluster states, which is the entanglement resource used in one-way quantum computation. (c). **Combinatorial approach to LOCC (local operations and classical communication) transformations in multipartite quantum states:** Here graph theoretic methods were applied to the analysis of pure maximally entangled quantum states distributed among multiple geographically separated parties [14, 15]. (d). **Braunstein, Ghosh and Severini approach:** Here, a single quantum state is represented by a graph [16, 17]. Combinatorial properties of a quantum mechanical state can be studied using this approach.

This work is in the spirit of the Braunstein et. al. approach. Representing a quantum state by a graph is beneficial for research in both quantum information theory as well as complex networks. Graphs provide a platform to visualize quantum states pictorially [18], such that different states have different pictographic representations [17] and some important unitary evolutions can also be represented by changes in their representations [19]. In this way, graphs form an intuitively appealing framework for quantum information and communication. On the other hand, measuring entropy and complexity of large, complex networks is a challenging part of network science. Correspondence between graphs and quantum states provide an insightful connection between the Shannon and von-Neumann entropy on the

*Electronic address: dutta.1@iitj.ac.in
†Electronic address: bibhas@maths.iitkgp.ernet.in
‡Electronic address: subhashish@iitj.ac.in
§Electronic address: srik@poornaprajna.org

one hand and, on the other, the complexity of networks [20, 21], details of which can be seen from [22–25]. This interconnection has also been exploited in quantum gravity and quantum spin networks [26].

A combinatorial graph $G = (V(G), E(G))$ is an ordered pair of sets $V(G)$ and $E(G)$, where $V(G)$ is called the vertex set and $E(G) \subseteq V(G) \times V(G)$ is the edge set. In this paper, we are concerned with simple graphs, which are graphs without multiple edges and loops. Between any two vertices there is a maximum of one edge. There is no edge linking a vertex to itself. An edge is denoted by $(i, j)$ which links the vertices $i$ and $j$. The adjacency matrix $A(G) = (a_{ij})$ associated with a simple graph $G$ is a binary (all elements are $0, 1$) symmetric matrix defined as

$$a_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

Thus, the order of $A(G)$ is $|V(G)|$ where, $|V(G)|$ denotes the number of elements of the vertex set, $V(G)$. The degree of a vertex $u$ is the number of edges incident to it, denoted by $d_G(u)$. The degree matrix $D(G)$ of $G$ is the diagonal matrix of order $|V(G)|$. Its $i$-th diagonal entry is the degree of the $i$th vertex of $G$, $i = 1, 2, \dots, |V|$. Two simple graphs $G_1$ and $G_2$ are isomorphic if there exists a bijective map $f : V(G_1) \to V(G_2)$, such that $(i, j) \in E(G_1)$ if and only if $(f(i), f(j)) \in E(G_2)$. When $G_1$ and $G_2$ are isomorphic there is a permutation matrix $P$ such that $A(G_1) = P^T A(G_2) P$.

In quanutm mechanics a density matrix $\rho$ is a positive semidefinite Hermitian unit-trace matrix. Familiar positive semidefinite matrices related to a graph are the combinatorial Laplacian matrix $L(G) = D(G) - A(G)$ [2], the signless Laplacian matrix $Q(G) = D(G) + A(G)$ [27] and the normalised Laplacian matrix $M(G)$ [28, 29]. In this work, we are concerned with the density matrices corresponding to $L(G)$ and $Q(G)$ only. They are defined as [17]

$$\rho_l(G) = \frac{L(G)}{\text{Trace}(L(G))} \text{ and } \rho_q(G) = \frac{Q(G)}{\text{Trace}(Q(G))}.$$

For any two isomorphic graphs $G_1$ and $G_2$,

$$L(G_1) = P^T L(G_2) P \qquad \text{and} \qquad Q(G_1) = P^T Q(G_2) P.$$

$$\Rightarrow \rho_l(G_1) = P^T \rho_l(G_2) P \qquad \text{and} \qquad \rho_q(G_1) = P^T \rho_q(G_2) P.$$

Throughout this paper we shall denote a general density matrix by $\rho$, while $\rho_l(G)$ and $\rho_q(G)$ are specific density matrices as defined above, collectively written as $\rho(G)$.

Here, we are concerned with bipartite systems distributed between two parties $A$ and $B$. It is well known that a state of such a system, represented by the density matrix $\rho$, is separable if and only if it can be represented as a convex combination of product states, i.e., there are two sets of density matrices $\{\rho_k^{(A)} : \text{ order}(\rho_k^{(A)}) = m\}$ and $\{\rho_k^{(B)} : \text{ order}(\rho_k^{(B)}) = n\}$ corresponding to $A$ and $B$ respectively, such that,

$$\rho = \sum_k p_k \rho_k^{(A)} \otimes \rho_k^{(B)}; \sum_k p_k = 1, \; p_k \geq 0.$$

Here and below, $\otimes$ denotes tensor product of matrices [30]. Trivially, the dimension of $\rho$ is $mn$. The state corresponding to $\rho$ is called entangled if it is not separable [31]. If $k = 1$ in the above equation, $\rho$ is called a pure state. Else, it is a mixed state which is a probabilistic mixture of different pure states. Detection of entangled states, known as the "quantum separability problem" (QSP), is one of the fundamental problems of the quantum information theory [32] due to its wide applications in various quantum communication and information processing tasks. The Peres-Horodecki criterion [33–35], also known as the positive partial transpose (PPT) criterion, provides a necessary condition for separability. It also provides a sufficient condition for systems of dimension $2 \times 2$ and $2 \times 3$. However, sufficiency for higher dimensional systems requires in general other techniques, like entanglement witness. As $\rho$ is a matrix of order $mn$, it can be written as an $m \times m$ block matrix with each block of size $n \times n$. The partial transpose corresponding to $B$, denoted by $\rho^{T_B}$, is obtained by taking individual transpose of each block [35]. The PPT criterion states that for any separable state, $\rho^{T_B}$ is a positive semi-definite matrix [33]. However, the converse is true only for bipartite systems of dimensions $2 \times 2$ and $2 \times 3$ [34]. There are a number of other separability critera [31].

The graph theoretic approach to solving QSP has generated a lot of interest in the last decade after the seminal paper [16]. This approach is beneficial as it is more efficient for mixed states. The state $\rho(G)$ is pure if it consists of a single edge; otherwise it is mixed [16, 17]. The separability of bipartite quantum states corrsponding to random graphs are considered in [36]. Some families of graphs were invented for which separability can be tested easily [37]. The idea of entangled edges [16, Section 4.3] was generalised in [38]. Motivated by the PPT criteria, the QSP problem for

$\rho_l(G)$ was considered in [39], where, the concept of partial transpose was introduced graph theoretically. It introduced the degree criteria as the condition for separability. However, the degree criteria failed to detect bound entangled states, that is, entangled states with positive partial transpose. Thus, finding sufficient conditions on graphs that can generate separable states is a current topic of interest in the literature. A class of graphs which produce $2 \times p$ separable quantum states were identified in [40]. The degree criterion was generalised for tripartite states in [41]. In [42–44] QSP for higher dimensional states were addressed. For some particular class of graphs, the properties of corresponding quantum states were discussed in [45, 46]. An interesting fact, already discussed in the literature regarding QSP, is that separability of $\rho(G)$ does not depend on graph isomorphism. Two isomorphic graphs may correspond to quantum states with different separability properties [16, 39, 44]. This is contradictory to our classical world phenomena, wherein any two isomorphic graphs possess the same properties.

In [39], the degree criterion was shown to be equivalent to the PPT criterion. Hence, a stronger criterion for separability than the degree criterion is essential. Inspired by the degree criteria, in this paper, we define degree symmetric graphs. The motivation for this is that entanglement of $\rho_l(G)$ and $\rho_q(G)$ may depend on some symmetry hidden in the graph. Inspired by this idea we define here a notion of partial symmetry. We generalise the result of [40] to partially symmetric graphs. Then we derive a class of partially symmetric graphs which produce separable quantum states $\rho_l(G)$ and $\rho_q(G)$ of dimension $m \times n$. To the best of our knowledge, there are no sufficient conditions till date for separability of $m \times n$ systems arising from graphs. How to generate bigger graphs providing separable states from smaller graphs? We define a graph product $G \bowtie H$ for a simple graph $G$ and a partially symmetric graph $H$ which corresponds to separable bipartite states.

We collect our ideas related to separability and partially symmetric graphs in the Section 2. Here we also introduce the concept of multi-layered system in the context of graphs. In Section 3, we use graph isomorphism as an entanglement generator. As a by-product of the separability criteria, we propose some graph isomorphisms, which are non-local in nature, to generate entanglement from a given partially symmetric graph. Finally, we provide an example of an entangled state generated by employing this non-local operation on a partially symmetric graph which represents separable states. Thus, we conclude from this example that non-local operations are not limited to the use of CNOT gate operations on separable states, as is observed in quantum information theory. We then make our conclusions and bring out some open problems arising from this work.

## II. PARTIAL SYMMETRIC GRAPHS AND SEPARABILITY

This section begins with the creation of layers in a graph $G$. It partitions density matrices $\rho(G)$ into blocks. We also define graph theoretical partial transpose (GTPT), the graph theoretical analogue of partial transpose. This is an equivalence relation on the set of all graphs. GTPT equivalent graphs preserve the separability property. Next, we define partial symmetric graphs. A sufficiency condition is provided for separability of states which arise from partially symmetric graphs. We also define a product operation for two graphs such that the density matrices corresponding to the resultant graph represent separable states.

Let the vertex set of the graph $G$, $V(G)$, with $mn$ number of vertices be labelled by integers $1, 2, \ldots, mn$. Then partition $V(G)$ into $m$ layers with $n$ vertices in each layer. Let the layers be $C_1, C_2, \ldots, C_m$ where $C_i = \{v_{i,1}, v_{i,2}, \ldots v_{i,n}\}$ and $v_{i,k} = ni + k$. This allows $A(G)$ to be partitioned into blocks as follows.

$$A(G) = \begin{bmatrix} A_1 & A_{1,2} & \ldots & A_{1,m} \\ A_{2,1} & A_2 & \ldots & A_{2,m} \\ \vdots & \vdots & \vdots & \vdots \\ A_{m,1} & A_{m,2} & \ldots & A_m \end{bmatrix}, \tag{1}$$

where $A_{i,j}, i \neq j$ and $A_i$ are matrices of order $n$. $A_{i,j}, i \neq j$ represents edges between $C_i$ and $C_j$. $A_i$ represents edges between vertices of $C_i$. Trivially, $A_i^T = A_i$ and $A_{i,j}^T = A_{j,i}$ for all $i \neq j$. Observe that $A_{i,j}$ need not be symmetric. Throughout this article, $G$ is a simple graph with standard labelling on the vertex set $V(G) = \{1, 2, \ldots, mn\}$ with layers as described above.

This article deals with quantum entanglement of bipartite states of dimension $m \times n$ which arise from simple graphs of $mn$ vertices. We mention that the bipartition does not exist a-priori in the graph, but is induced by the above layering. We wish to understand how the two abstract "particles", created by this induction based on vertex labellings are related to $G$. $V(G)$ is arranged as a matrix of dots as follows.

$$\begin{array}{lllll} C_1 = & \bullet_{v_{1,1}} & \bullet_{v_{1,2}} & \cdots & \bullet_{v_{1,n}} \\ C_2 = & \bullet_{v_{2,1}} & \bullet_{v_{2,2}} & \cdots & \bullet_{v_{2,n}} \\ \vdots & & & & \\ C_m = & \bullet_{v_{m,1}} & \bullet_{v_{m,2}} & \cdots & \bullet_{v_{m,n}} \end{array} \tag{2}$$

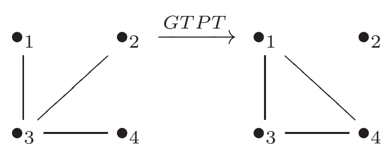
Effectively, one particle, of dimension $n$, is assumed to correspond to horizontal direction, whilst another particle, of dimension $m$, corresponds to the perpendicular direction. Thus, the first and second indices of every vertex label $A_{j,k}$ comes from the vertical and horizontal particles, respectively. More particles can be induced in the system in different orthogonal directions by drawing $G$ in an orthogonal higher dimensional structure, which will be explored elsewhere. In the analogous construction for a 3-partite system of dimension $lmn$, we can arrange the entries of $A_{j,k}$ as a three-dimensional stack, with the vertical layer of height $l$. Then the entries $A_{j,k}$ $(j = 1, \cdots, m; k = 1, \cdots, n)$ will be on the "ground" layer, with the next layer having the entries $A_{j,k}$ $(j = m+1, \cdots, 2m; k = n+1, \cdots, 2n)$ and in general the $r$th layer $(1 \leq r \leq l)$ having the entries $A_{j,k}$ $(j = (r-1)m+1, \cdots, rm; k = (r-1)n+1, \cdots, rn)$. Note that this scheme can be introduced for any number of induced particles, but the simple assignment of direction to particles as "vertical" and "horizontal" will no longer be possible for three or more particles.

Let us return to the bipartite case. As defined in [39, 40], we recall that partially transposed graph $G'$ is obtained by employing the algebraic partial transposition to the adjacency matrix of a given graph $G$. This idea is equivalent to partial transpose on the 2-nd party in a bipartite systems density matrix. For convenience in dealing with our labelling of the vertices in the graph $G$, we reformulate the definition of partially transposed graph by introducing it as a by-product of the following combinatorial operation.

**Definition 1.** *Graph theoretical partial transpose (GTPT) is an operation on the graph G replacing all existing edges* $(v_{i,k}, v_{j,l}), k \neq l, i \neq j$ *by* $(v_{i,l}, v_{j,k})$*, keeping all other edges unchanged.*

Thus, GTPT generates a new simple graph $G' = (V(G'), E(G'))$ from a given simple graph $G = (V(G), E(G))$ where $V(G') = V(G)$ with the labelling unchanged. Note that, $G$ can also be constructed from $G'$ by GTPT as, $(G')' = G$. We call $G$ and $G'$ as GTPT equivalent. It is easy to verify that $A(G') = A(G)^{T_B}$ and hence $|E(G)| = |E(G')|$.

**Example 1.** *The GTPT of the star graph with four vertices is depicted below.*

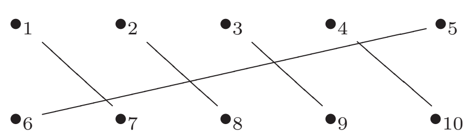



The Example 1 establishes that GTPT of a connected graph need not be connected. Also, it changes the degree sequence of the graph. A relevant question here is: does there exist a graph for which the degree sequence remains invariant under GTPT? Inspired by the degree criteria introduced in [16, 39], we define degree symmetric graphs as follows.

**Definition 2.** *A graph $G$ is called degree symmetric if $d_G(u) = d_{G'}(u)$ for all $u \in V(G) = V(G')$.*

Thus, for a degree symmetric graph, the degree sequence of the graph is preserved under GTPT. The following is an example of a degree symmetric graph.

**Example 2.** *[16]*




It was conjectured in [16] that $\rho_l(G)$ is a separable bipartite state in any dimension if and only if $G$ and $G'$ have the same degree sequence. In other words, $\rho_l(G)$ is separable if and only if $G$ is a degree symmetric graph. Later the conjecture was proved to be false in [39]. An example of a degree symmetric graph $G$ was provided for which $\rho_l(G)$ is entangled. It was established that PPT criteria is equivalent to the degree criteria for $\rho_l(G)$. However, the separability of $\rho_l(G')$ and $\rho_q(G')$ was not discussed there [39]. In this work we prove that degree symmetric graphs preserve the separability even after GTPT. This result can be stated as a theorem.

**Theorem 1.** *Separability of $\rho_l(G)$ implies the separability of $\rho_l(G')$ if and only if $G$ is degree symmetric. Similarly separability of $\rho_q(G)$ implies separability of $\rho_q(G')$ if and only if $G$ is degree symmetric.*

The proof can be found in the appendix.

Now we introduce the concept of partially symmetric graphs. This will play a central role in the development of the rest of the paper. Our aim is to make a more stringent condition of symmetry in a degree symmetric graph. We focus on symmetry in the partial transposition of the adjacency matrix of a graph and hence, define partially symmetric graphs (in analogy with "partial transpose") as follows.

**Definition 3.** *A graph $G$ is partially symmetric if $(v_{i,l}, v_{j,k}) \in E(G)$ implies $(v_{i,k}, v_{j,l}) \in E(G)$ $\forall$ $i, j, k, l, i \neq j$.*

In the above definition, $i$ and $j$ indicates layers $C_i$ and $C_j$ such that vertices $v_{i,l} \in C_i$ and $v_{j,k} \in C_j$. Suffixes $l$ and $k$ represents the relative positions of the vertices in the individual layers.

Note that, GTPT keeps a partial symmetric graph unchanged as, $A_{i,j} = A^T_{i,j}, D(G) = D(G')$. This leads to the following lemma.

**Lemma 1.** *Every partial symmetric graph $G$ is degree symmetric.*

The converse of the Lemma 1 need not be true. There are many graphs which are degree symmetric but not partially symmetric. For example, consider the graph depicted in Example 2.

The above lemma leads us to the next theorem. It is a sufficient condition for separability of density matrices arising from partial symmetric graphs. We mention that, this result generalizes the result of [40], where a similar result was obtained for a $2 \times n$ dimensional system.

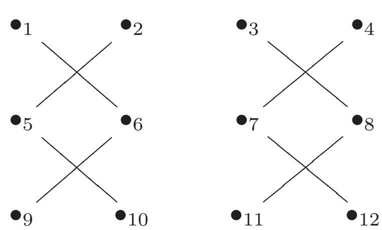
**Theorem 2.** *Let $G$ be a partially symmetric graph with the following properties.*

- *Between two vertices of any partition $C_i$ there is no edge. $(v_{i,l}, v_{i,k}) \notin E(G)$ for all $i, l, k$.*
- *Either there is no edge between vertices of $C_i$ and $C_j$, or $A_{i,j} = A_{k,l}$ for all $i, j, k, l, i \neq j$ and $k \neq l$.*
- *Degrees of all the vertices in a layer are same, i.e., $d_{C_i}(v_r) = d_{C_i}(v_s)$ for all $v_r, v_s \in C_i$, for all $i$.*

*Then $\rho(G)$ is separable i.e. $\rho(G) = \sum_i w_i \rho_A^i \otimes \rho_B^i, \sum_i w_i = 1$.*

Its proof is deferred to the appendix.

**Example 3.** *An example of a partially symmetric graph $H$ satisfying all the conditions of Theorem 2 is as follows.*

$H =$ 


Theorem 2 is a sufficient condition but not necessary. There are classes of partial symmetric graphs generating separable states without satisfying conditions of this theorem. Some of them will be discussed now.

Recall that, the union graph of two graphs $G = (V(G), E(G))$ and $H = (V(H), E(H))$ is defined as the new graph $G \cup H = (V(G) \cup V(H), E(G) \cup E(H))$ [1]. Let $G$ be a graph of order $n$ with vertex labelling $\{1, 2, \dots n\}$. Define, $mG = G \cup G \cup \cdots \cup G$ (union of $m$-copies of $G$) with vertex labelling $\{v_{j,k} : v_{j,k} = jn + k\}$. Note that, copies of $G$ form the layers of $mG$. There is no edge between two layers. Hence, $mG$ is trivially partially symmetric and it violates the 1-st condition of Theorem 2 which states that there will be no edge between two vertices located in the same layer. Interestingly, we will show now that $mG$ represents separable states. Observe that

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

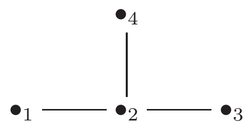
where, $I_m$ denotes the identity matrix of order $m$. Trivially, $\rho_l(mG) = \frac{L(mG)}{\text{trace}(L(mG))}$ and $\rho_q(mG) = \frac{Q(mG)}{\text{trace}(Q(mG))}$ are separable states. This result may be expressed as follows.

**Lemma 2.** *For any graph $G$, $\rho_l(mG)$ and $\rho_q(mG)$ represent separable bipartite states of dimension $m \times n$ w.r.t standard labelling on $mG$.*

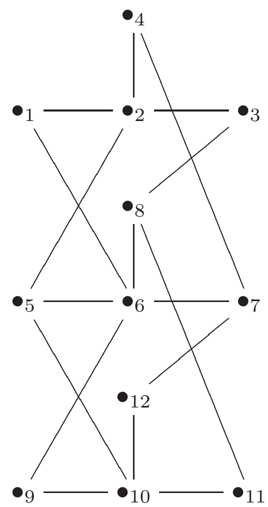
Note that, $G$ may not correspond to a separable state but $mG$ always represents a separable state. This lemma is significant as it suggest more general conditions for separability.

We define a new graph operation as follows. Consider a partially symmetric graph $H$ with $m$ different layers, each layer having $n$ number of vertices and $H$ satisfies all the conditions of Theorem 2, while $G$ is a simple graph with $n$ vertices. We define the new graph $G \bowtie H$ as the graph which is constructed by replacing each layer of $H$ by the graph $G$. Note that, $V(G \bowtie H) = V(H)$. An example which illustrates the operation $G \bowtie H$, is given below.

**Example 4.** *Consider the star graph $G$ with four vertices given by*




*and $H$ is a graph given in Example 3. Then the graph $G \bowtie H$ is as follows.*




Now we present some properties of $G \bowtie H$ where $G$ and $H$ are the graphs as discussed above.

$H$ satisfies all the conditions of theorem (2). Hence, there is no edge joining two vertices belonging to the same layer. This implies that the diagonal blocks of $A(H)$ are zero matrices. Graph $G$ is placed $m$ times on the layers of $H$. Thus all $m$ diagonal blocks of $A(G \bowtie H)$ are $A(G)$. Hence, we have the following lemma.

**Lemma 3.** $A(G \bowtie H) = A(mG) + A(H)$, *where $I_m$ is the identity matrix of order $m$.*

It is clear from the construction of $G \bowtie H$ that the degree of a vertex in $G \bowtie H$ is the sum of its degree in $H$ and its degree in $G$. Incorporating this in the expression of $A(G \bowtie H)$, we obtain the following result.

**Lemma 4.** $D(G \bowtie H) = D(mG) + D(H)$.

The above two lemmas together imply the structure of the Laplacian $L(G)$ and the signless Laplacian $Q(G)$, i.e., the structures of the density matrices $\rho_l(G)$ and $\rho_q(G)$.

**Lemma 5.** $L(G \bowtie H) = L(H) + L(mG)$ *and* $Q(G \bowtie H) = Q(H) + Q(mG)$.

*Proof.*

$$\begin{aligned}
L(G \bowtie H) &= D(G \bowtie H) - A(G \bowtie H) \\
&= I_m \otimes D(G) + D(H) - I_m \otimes A(G) - A(H) \\
&= I_m \otimes (D(G) - A(G)) + D(H) - A(H) \\
&= I_m \otimes L(G) + L(H) \\
&= L(H) + L(mG)
\end{aligned}$$

□

Similarly, $Q(G \bowtie H) = Q(H) + Q(mG)$.

All the above lemmas together indicate the separability of $G \bowtie H$.

**Theorem 3.** *$G \bowtie H$ represents a bipartite separable state of dimension $m \times n$.*

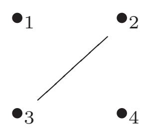
**Example 5.** *Consider the Werner state which is a mixture of projectors onto the symmetric and antisymmetric subspaces, with the relative weight $p_{sym}$ being the only parameter that defines the state.*

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

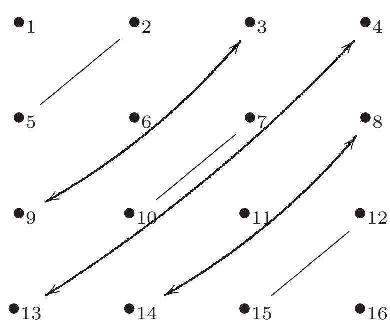
*where, $P_{sym} = \frac{1}{2}(1+P), P_{as} = \frac{1}{2}(1-P)$, are the projectors and $P = \sum_{ij} |i\rangle\langle j| \otimes |j\rangle\langle i|$ is the permutation operator that exchanges the two subsystems.*

*Only $\rho(d,0) = \frac{I-P}{d^2-d}$ is represented by a Laplacian matrix of simple graphs. For example, for $d = 2,3$ we have*

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

$\equiv$ 


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

$\equiv$ 


*It is easy to verify that these graphs are not degree symmetric and hence not partially symmetric. Further, these graphs represent entangled states.*

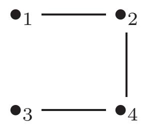
## III. A NON-LOCAL QUANTUM OPERATION ON GRAPHS

Observe that the definition of partially symmetric graphs relies on the labelling of the vertices. In fact, in the graph theoretic approach of interpretation of quantum states, it is well known that properties of a density matrix derived from a graph is vertex labelling contingent. A graph which represents a separable state corresponding to a vertex labelling, may also produce an entangled state for a different vertex labelling. In this section we describe graph isomorphism as a non-local operation to generate entanglement. We begin with an example.

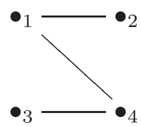
**Example 6.** *Let $G$ be a graph given by*



*It is easy to verify that the density matrix $\rho_l(G_1)$ corresponding to the graph $G_1$ with labelled vertices given below represents a separable state.*

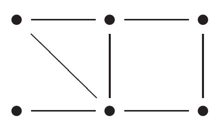



*Whereas, $\rho_l(G_2)$ represents an entangled state for the following graph $G_2$ with a different vertex labelling.*




It is evident that these graphs are isomorphic. It has also been proved that separability of $\rho_l(G)$ when $G$ is a completely connected simple graph does not depend on vertex labelling, and the states $\rho_l(G)$ corresponding to a star graph with respect to any labelling are entangled [Section 6, [16]]. In [16], it is also asked if there exist any other graphs which have this property. We mention that, in the search of partially symmetric graphs, we found one more graph given below, having the property that, for any vertex labelling, the graph represents an entangled state. In fact, this graph has no vertex labelling for which it can be made a partially symmetric graph.

**Example 7.** *The graph $G$ for which no vertex labelling produces a partially symmetric graph.*



(3)

Based on the above observations, we classify the set of all graphs with a fixed number of vertices into the following three classes.

1. **E-graph:** Independent of vertex labelling, all quantum states related to this graph are **E**ntangled.
2. **S-graph:** Independent of vertex labelling, all quantum states related to this graph are **S**eparable.
3. **ES-graph:** Quantum states related to some of the vertex labelling are **E**ntangled and others are **S**eparable.

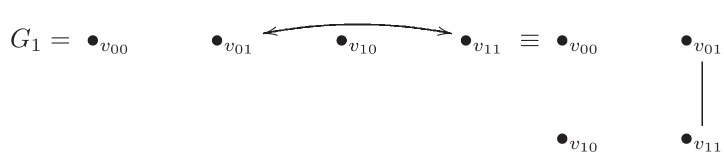
Obviously the completely connected graph is a S-graph, the star graph is an E-graph and the graph in Example 7 is an E-graph.

In this section, we are interested in ES-graphs. These graphs provide a platform for generating entanglement using graph isomorphism as a non-local operation. Changing the vertex labelling on a graph representing a separable state, generates its isomorphic copy representing an entangled state. It is proved in the literature [16, 17], that any graph with more than one edge represents a mixed state. Hence, graph isomorphism acts as an entanglement generator on both pure and mixed states. For example, the isomorphism $\phi : V(G_1) \to V(G_2)$ defined as

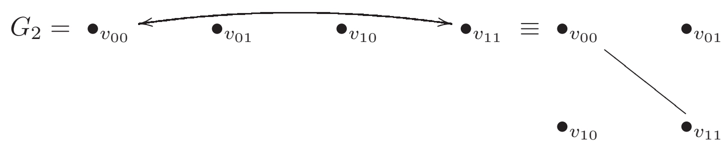
$$\phi(1) = 2, \phi(2) = 1, \phi(3) = 3, \phi(4) = 4$$

act as an mixed state entanglement generator in Example 6. The following example of pure state entanglement generator may be of interest to the quantum information community.

**Example 8.** *The following graph represents the density matrix of the separable state $\frac{1}{\sqrt{2}} |0 + 1\rangle |1\rangle$*



*We define a graph isomorphism $\phi$ acting on $G_1$. $\phi(v_{00}) = v_{00}, \phi(v_{01}) = v_{01}, \phi(v_{10}) = v_{11}, \phi(v_{11}) = v_{10}$ . It generates the graph*




*Graph $G_2$ represents the Bell state $\frac{1}{\sqrt{2}}|00+11\rangle$ [17]. Note that graph $G_1$ was partially symmetric but graph $G_2$ is not. The graph isomorphism $\phi$ here acts in a fashion analogous to a CNOT gate. Note that, every graph isomorphism corresponds to permutation similar matrices (for example, Laplacian and signless Laplacian matrices) associated with the graph and its isomorphic copy. This has a resemblance to a CNOT gate which is itself a permutation matrix. At the end of this section we present an example where the permutation matrix is different from the CNOT operation. Thus, we may conclude that graph isomorphisms are in general entangling operations.*

These examples inspire a number of questions for further investigation. For instance, which isomorphisms will act as an entanglement generator? In the remaining part of this work we try to address this question.

**Definition 4.** *In a graph $G$, partial degree of a vertex $v_{i,k} \in C_i$, w.r.t the layer $C_j$ is denoted by $ld_{C_j}(v_{i,k})_G$ and defined by the number of edges from $v_{i,k}$ to the vertices of $C_j$. When no confusion occurs, instead of $ld_{C_j}(v_{i,k})_G$, we may write $ld_{C_j}(v_{i,k})$.*

**Definition 5.** *In a graph $G$, a vertex $v_{i,k}$ is internally related to vertex $v_{i,l}$ in $C_i$ w.r.t layer $C_j$ if $(v_{i,k}, v_{j,l})$ and $(v_{i,l}, v_{j,k}) \in E(G)$.*

$ld_{C_j}(v_{i,k})$ = number of vertices internally related to $v_{i,k}$ in $C_i$ w.r.t $C_j$ for a partial symmetric graph.

**Definition 6.** *$G$ is called partially asymmetric if $\exists\ (v_{i,k}, v_{j,l}) \in E(G), i \neq j, k \neq l$ such that $(v_{i,l}, v_{j,k}) \notin E(G)$.*

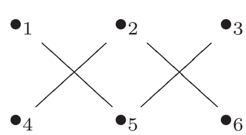
Incidence set of $v \in V(G)$ is $I_G(v) = \{w : (w, v) \in E(G)\}$, that is, set of all vertices incident to vertex $v$. Incidence interchange between two vertices $u, v$, denoted by $u \overset{i}{\leftrightarrow} v$, is a graphical operation to construct a graph $H$ from $G$, defined as follows.

$$u \overset{i}{\leftrightarrow} v \equiv \begin{cases} I_H(u) = I_G(v) \\ I_H(v) = I_G(u) \end{cases} . \tag{4}$$

This operation can generate mixed entangled states from a mixed separable state, as described later. Note that this is not a physical operation between two pre-existing particles, but a purely mathematical operation between two "formal" particles induced by how we biparition the graph. Hence there is no contradiction with the physical principle of non-increase of entanglement under LOCC (local operations and classical communication). This form of entanglement creation is reminiscent of the idea put forth in [47], that the degrees of freedom and hence entanglement are observer-induced.

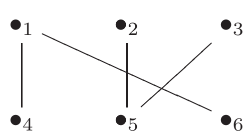
Note that $H$ is a layered graph and is also isomorphic to $G$. Let us see an example.

**Example 9.** *Initially we consider a graph $G$ with the following labels and layers $C_1 = \{1, 2, 3\}$ and $C_2 = \{4, 5, 6\}$*




(5)

*$H$ is generated from $G$ by graphical operation $1 \leftrightarrow 2$, namely:*




(6)

Note that in the above example initially $G$ was a partially symmetric graph. $dl_{C_1}(1) = 1$ but $dl_{C_1}(2) = 2$. After interchanging the vertex labellings of 1 and 2 the new graph is $H$, which is partially asymmetric. It can be generalised for an arbitrary partially symmetric graph.

Let in a partially symmetric graph $G$, $ld_{C_j}(v_{i,k}) \geq ld_{C_j}(v_{i,l})$, then $ld_{C_j}(v_{i,k}) - ld_{C_j}(v_{i,l}) \geq 1$. $ld_{C_j}(v_{i,k})$ and $ld_{C_j}(v_{i,l})$ represent number of internally related vertices in $C_i$ of $v_{i,k}$ and $v_{i,l}$ w.r.t $C_j$, respectively. Thus, there exists at least one vertex $v_{i,s}$, internally related to $v_{i,k}$ but not with $v_{i,k}$. After interchanging vertex labellings there will be at least one edge incident to $v_{i,s}$ without any complement as the complement edge is misplaced by interchange. Hence, the new graph $H$, isomorphic to $G$, is partially asymmetric. This can be expressed as a lemma.

**Lemma 6.** *Assume, $ld_{C_j}(v_{i,k}) \neq ld_{C_j}(v_{i,l})$ in a partially symmetric graph $G$. Graph $H$ is generated after interchanging vertex labellings of the vertices $v_{i,l}$ and $v_{i,k} \in E(G)$. Then $H$ is partially asymmetric.*

Also, $(v_{i,s}, v_{j,l}) \notin E(G) \Rightarrow$ complement of $(v_{i,l}, v_{j,k}) \notin E(H)$, but $(v_{i,l}, v_{j,k}) \in E(H)$. Trivially, $H$ is not partially symmetric.

**Lemma 7.** *Let $(v_{i,l}, v_{j,k}) \in E(G), i \neq j, l \neq k$; but $(v_{i,s}, v_{j,l}) \notin E(G)$ for some $s$, where $G$ is a partially symmetric graph. Interchange of vertex labellings of $v_{i,s}$ and $v_{i,l}$ will generate partial asymmetric graph $H$.*

This change of labelling may not generate partial asymmetry in all the cases. Suppose any two vertices of $C_i$ are not internally related w.r.t $C_j$. Hence, any edge between vertices of $C_i$ and $C_j$ is of the form $(v_{i,k}, v_{j,k})\ \forall\ k = 1, 2, \dots n$. Consider any two vertices of $C_i$, say $v_{i,l}$ and $v_{i,k}$. Interchange of vertex labellings of these two vertices will generate new edges $(v_{i,l}, v_{j,k})$ and $(v_{i,k}, v_{j,l})$. This implies partial symmetry in the new graph. We may write it as a lemma.

**Lemma 8.** *Suppose any two vertices of $C_i$ are not internally related w.r.t $C_j$. Also assume that $ld_{C_j}(v_{i,l}) = ld_{C_j}(v_{i,k})\ \forall\ k, l = 1, 2, \dots n$. Then interchange of vertex labellings of any two vertices of $C_i$ will not generate partial asymmetry.*

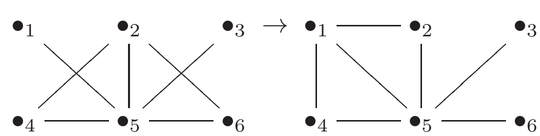
Graph isomorphism is an equivalence relation on the set of all simple graphs, which forms disjoint equivalence classes. Let $\mathcal{G}$ be one such class and $\mathcal{L}$ be set of all isomorphisms on $\mathcal{G}$. $\circ$ is composition of mappings.

Trivially $(\mathcal{L}, \circ)$ forms a group which is a permutation group over $\#(V(G))$ elements. For an ES graph $\mathcal{G} = \mathcal{E} \cup \mathcal{S}, \mathcal{E} \cap \mathcal{S} = \phi, \mathcal{E} \neq \phi, \mathcal{S} \neq \phi$. $\mathcal{E}$ and $\mathcal{S}$ are subclasses of $\mathcal{G}$ consisting of all graphs providing entangled and separable states respectively.

Let $\mathcal{L}_e$ and $\mathcal{L}_s$ be the group of all graph isomorphisms acting on $\mathcal{E}$ and $\mathcal{S}$. Trivially $(\mathcal{L}_e, \circ)$ and $(\mathcal{L}_s, \circ)$ also form groups. Entanglement generators are invertible mappings from $(\mathcal{L}_s, \circ)$ to $(\mathcal{L}_e, \circ)$.

**Remark 1.** *In example 9, the graphical operation $1 \leftrightarrow 2$ represents a quantum entanglement generator which transforms the separable states $\rho(G)$ to entangled states $\rho(H)$.*

**Example 10.** *It is clear to us that graph isomorphism acts as a global unitary operator and it is capable to generate mixed entangled state from mixed separable state. Consider two isomorphic graphs.*




*Corresponding permutation is*

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 6 & 1 & 3 & 4 & 5 & 2 \end{pmatrix}$$

*The permutation matrix is*

$$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

*This operator acts as an entanglement generator. Density matrices corresponding to the first graph is separable but for the second graph $\rho_l$ and $\rho_q$ both are entangled.*

## IV. CONCLUSION AND OPEN PROBLEMS

The quantum separability problem is an important and difficult open problem in quantum information theory. For quantum states related to simple combinatorial graphs some sufficiency conditions are available in the literature. For bipartite systems they were applicable for some special cases of $2 \times p$ systems. Here, we have generalised these results to $m \times n$ systems.

In another direction, ourwork proposes the use of of graph isomorphisms as entanglement generators, which can generate mixed entangled states from mixed separable states. Note that, these isomorphisms are formal operations, in contrast to physical operations like LOCC (local operations and classical communication), which cannot generate entanglement. As mentioned above, combinatorial graphs enable us to visualize changes of quantum states under a particular quantum operation pictorially. In this context, graph isomorphisms pictorially depict certain actions that lead to entanglement generation. Finally, this work initiates a number of problems or directions for future investigations: (a). Can a combinatorial criterion be defined to detect entangled states arising from graphs? Can the quality of entanglement be defined by using the partially asymmetric graphs? (b). Can the formulation of partially symmetric graphs be generalized for weighted graphs that may possibly open up combinatorial formulation of separable states? (c). Generalization of the bipartite separability criteria arising from partially symmetric graphs to the case of multipartite states? (d). Further investigations are required for the identification of ES graphs (See example 7). Precisely, when is a graph an ES graph? How much entanglement can be generated from a separable copy of an ES graph using graph isomorphism? Here the results of [14] should be leveraged.

We hope that this work is a contribution to the graphical representation of quantum mechanics, in general and the separability problem, in particular.

### Acknowledgement

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### Appendix

**Proof of Theorem 1:**

*Proof.* Let $G$ be a graph and $\rho_l(G)$ separable. Then

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

$$\begin{aligned}
\rho_l(G') &= \rho_l(G)^{T_B} - \frac{1}{\mathrm{Trace}(L(G))}(D(G) - D(G')) \\
&= \sum_i p_i \rho_i^A \otimes (\rho_i^B)^{T_B} - \frac{1}{\mathrm{Trace}(L(G))}(D(G) - D(G')) \\
\rho_l(G')^{T_B} &= \sum_i p_i \rho_i^A \otimes \rho_i^B - \frac{1}{\mathrm{Trace}(L(G))}(D(G) - D(G'))\ [\because (D(G))^{T_B} = D(G).]
\end{aligned}$$

Thus, the desired result follows for $\rho_l(G)$.
Similarly, $\rho_q(G')^{T_B} = \sum_i p_i \rho_i^A \otimes \rho_i^B + \frac{1}{\mathrm{Trace}(Q(G))}(D(G) - D(G'))$, assuming, $\rho_q(G') = \sum_i p_i \rho_i^A \otimes \rho_i^B$. This completes the proof. □

**Proof of theorem 2:**

*Proof.* Since $A_{i,j}$ is a symmetric matrix, the spectral decomposition of $A_{i,j}$ is given by $A_{i,j} = \sum_r \lambda_r u_r u_r^t$ where $\{u_r : r = 1 : n\}$ is a complete set of orthonormal eigenvectors corresponding to the eigenvalues $\lambda_r, r = 1 : n$ of $A_{i,j}$. For $A_{i,j} = 0, A_{i,j} = \sum_r 0.u_r u_r^t$. Since $u_r, r = 1 : n$ are normalised eigenvectors, $u_r u_r^t$ is a trace 1 positive semi-definite matrix for each $r$. Since there are no edges between any two vertices n any layer $C_i$, $A_i = 0$ for all $i$. Further, $D_i = diag\{d_i\} = d_i I$ since $A_{i,j} = A_{k,l}$ for all $i, j, k, l, i \neq j$ and $k \neq l$.
Then

$$\begin{aligned}
L(G) &= \begin{bmatrix} d_0.I & A_{0,1} & A_{0,2} & \dots & A_{0,(m-1)} \\ A_{0,1} & d_1.I & A_{0,2} & \dots & A_{0,(m-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{0,(m-1)} & A_{1,(m-1)} & A_{2,(m-1)} & \dots & d_{m-1}.I \end{bmatrix} \\
&= \begin{bmatrix} d_0 \sum_r u_r u_r^t & \sum_r \lambda_r u_r u_r^t & \sum_r \lambda_r u_r u_r^t & \dots & \sum_r \lambda_r u_r u_r^t \\ \sum_r \lambda_r u_r u_r^t & d_1 \sum_r u_r u_r^t & \sum_r \lambda_r u_r u_r^t & \dots & \sum_r \lambda_r u_r u_r^t \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_r \lambda_r u_r u_r^t & \sum_r \lambda_r u_r u_r^t & \sum_r \lambda_r u_r u_r^t & \dots & d_{(m-1)} \sum_r u_r u_r^t \end{bmatrix} \\
&= \sum_r \begin{bmatrix} d_0 & \lambda_r & \lambda_r & \dots & \lambda_r \\ \lambda_r & d_1 & \lambda_r & \dots & \lambda_r \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \lambda_r & \lambda_r & \lambda_r & \dots & d_{m-1} \end{bmatrix} \otimes u_r u_r^t \\
&= \sum_r B(r) \otimes u_r u_r^t,
\end{aligned}$$

where $B(r) = \begin{bmatrix} d_0 & \lambda_r & \lambda_r & \dots & \lambda_r \\ \lambda_r & d_1 & \lambda_r & \dots & \lambda_r \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \lambda_r & \lambda_r & \lambda_r & \dots & d_m \end{bmatrix}$. Note that $A_{i,j} = 0 \Rightarrow b_{i,j} = 0$. Now we want to show $B$ is a positive semidefinite matrix.
Note that the spectral radius of $A_{i,j} \leq \|A_{i,j}\|_\infty$, where $\|A_{i,j}\|_\infty$ is the subordinate matrix norm defined by $\|A_{i,j}\|_\infty = \max_i \sum_{j=1}^n |a_{i,j}|$. Besides, $d_i = \sum_{k=0}^{m-1} \max_i \sum_{j=1}^n |a_{i,j}| = m \max_i \sum_{j=1}^n |a_{i,j}|$. Then, $(m-1)\lambda_r \leq (m-1) \times ($ Spectral radius of $A_{i,j}) \leq d_i\ \forall\ i$. Hence, $B$ is a diagonally dominant symmetric matrix with all positive entries. So $B$ is a positive semidefinite matrix. Hence $\rho_l(G)$ is separable. Similarly the result follows for $\rho_q(G)$. □


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