Bipartite separability and nonlocal quantum operations on graphs

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(Received 25 February 2016; published 5 July 2016)

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-theoretic counterpart of the familiar positive partial transpose criterion for separability, although there are entangled states with positive partial transpose for which the 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 that lack the property of partial symmetry. 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.

DOI: 10.1103/PhysRevA.94.012306

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 sciences, and systems biology [5], as well as in communications and information systems [6]. It is also used to address foundational aspects of different branches of mathematics and physics [7]. Combinatorial graphs have been used in quantum mechanics and information theory [8] in four different ways: (a) In the quantum graph approach, a differential or pseudodifferential 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) In the graph state 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) In the combinatorial approach to local operations and classical communication (LOCC) transformations in multipartite quantum states, the graph-theoretic methods are applied to the analysis of pure maximally entangled quantum states distributed among multiple geographically separated parties [14,15]. (d) In the approach of Braunstein *et al.*, 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 and 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. The correspondence between graphs and quantum states provides an insightful connection between the Shannon and von Neumann entropies on the one hand and the complexity of networks [20,21] on the other, the details of which can be found in [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 $d_G(u)$.

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The degree matrix $D(G)$ of G is the diagonal matrix of order $|V(G)|$. Its ith diagonal entry is the degree of the ith vertex of G, $i = 1,2,\dots,|V|$. Two simple graphs G_1 and G_2 are isomorphic if there exists a bijective map $f : V(G_1) \rightarrow V(G_2)$ 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 quantum mechanics a density matrix ρ 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 normalized 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]

$$\rho_l(G) = \frac{L(G)}{\mathrm{Tr}[L(G)]}, \quad \rho_q(G) = \frac{Q(G)}{\mathrm{Tr}[Q(G)]}.$$

For any two isomorphic graphs G_1 and G_2,

$$L(G_1) = P^T L(G_2)P, \quad Q(G_1) = P^T Q(G_2)P,$$
$$\Rightarrow \rho_l(G_1) = P^T \rho_l(G_2)P, \quad \rho_q(G_1) = P^T \rho_q(G_2)P.$$

Throughout this paper we denote a general density matrix by ρ, 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 ρ, 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 $\{\rho_k^{(A)} : O(\rho_k^{(A)}) = m\}$ and $\{\rho_k^{(B)} : O(\rho_k^{(B)}) = n\}$ corresponding to A and B, respectively, such that

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

Here and below $\otimes$ denotes the tensor product of matrices [30]. Trivially, the dimension of ρ is mn. The state corresponding to ρ is called entangled if it is not separable [31]. If $k = 1$ in the above equation, ρ is called a pure state; otherwise it is a mixed state that 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 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 dimensions 2×2 and 2×3. However, sufficiency for higher-dimensional systems requires in general other techniques, like an entanglement witness. As ρ 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 ρ^{T_B}, is obtained by taking the individual transpose of each block [35]. The PPT criterion states that for any separable state, ρ^{T_B} is a positive-semidefinite matrix [33]. However, the converse is true only for bipartite systems of dimensions 2×2 and 2×3 [34]. There are a number of other separability criteria [31].

The graph-theoretic approach to solving the QSP has generated a great deal of interest in the past decade after the seminal paper by Braunstein *et al.* [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 corresponding to random graphs is considered in [36]. Some families of graphs were invented for which separability can be tested easily [37]. The idea of entangled edges [16] was generalized in [38]. Motivated by the PPT criterion, the QSP problem for $\rho_l(G)$ was considered in [39], where the concept of a partial transpose was introduced graph theoretically. It introduced the degree criterion as the condition for separability. However, the degree criterion failed to detect bound entangled states, that is, entangled states with a 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 that produce $2 \times p$ separable quantum states was identified in [40]. The degree criterion was generalized for tripartite states in [41]. In [42–44] the QSP for higher-dimensional states was 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 the QSP, is that the 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 criterion, 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 generalize the result of [40] to partially symmetric graphs. Then we derive a class of partially symmetric graphs that produce separable quantum states $\rho_l(G)$ and $\rho_q(G)$ of dimension $m\times n$. 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 that corresponds to separable bipartite states.

We collect our ideas related to separability and partially symmetric graphs in Sec. II. Here we also introduce the concept of a multilayered system in the context of graphs. In Sec. III we use graph isomorphism as an entanglement generator. As a by-product of the separability criterion, we propose some graph isomorphisms, which are nonlocal in nature, to generate entanglement from a given partially symmetric graph. Finally, we provide an example of an entangled state generated by employing this nonlocal operation on a partially symmetric graph that represents separable states. Thus, we conclude from this example that nonlocal operations are not limited to the use of CNOT gate operations on separable states, as is observed in quantum information theory. In Sec. IV we summarize and discuss some issues 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 the graph-theoretic partial transpose (GTPT), the graph-theoretic analog of the partial transpose. This is an equivalence relation on the set of all graphs. The GTPT equivalent graphs preserve the separability property. Next we define partial symmetric graphs. A sufficiency condition is provided for separability of states that 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 the number of vertices mn be labeled by integers $1,2,\ldots,mn$. Then $V(G)$ is partitioned into m layers with n vertices in each layer. Let the layers be $C_1,C_2,\ldots,C_m$, where $C_i = \{v_{i,1},v_{i,2},\ldots,v_{i,n}\}$ with $v_{i,k} = ni + k$. This allows $A(G)$ to be partitioned into blocks as follows:

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

where $A_{i,j}$ $(i \neq j)$ and A_i are matrices of order n. Here $A_{i,j}$ $(i \neq j)$ represents edges between C_i and C_j and 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 labeling 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 $m \times n$ that 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 labels, are related to G. Here $V(G)$ is arranged as a matrix of dots as follows:

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

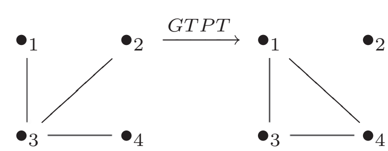
Effectively, one particle, of dimension n, is assumed to correspond to the horizontal direction, while another particle, of dimension m, corresponds to the perpendicular direction. Thus, the first and second indices of every vertex label $A_{j,k}$ comes from the vertical and horizontal particles, respectively. 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 three-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 $A_{j,k}$ $(j = 1,\ldots,m; k = 1,\ldots,n)$ will be on the ground layer, with the next layer having the entries $A_{j,k}$ $(j = m+1,\ldots,2m; k = n+1,\ldots,2n)$ and in general the rth layer $(1 \leqslant r \leqslant l)$ having the entries $A_{j,k}$ $[j = (r-1)m+1,\ldots,rm; k = (r-1)n+1,\ldots,rn]$. 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 the 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 a partial transposition on the second party in a bipartite system density matrix. For convenience in dealing with our labeling of the vertices in the graph G, we reformulate the definition of a partially transposed graph by introducing it as a by-product of the following combinatorial operation.

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

Thus, the 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 labeling unchanged. Note that G can also be constructed from G' by the GTPT as $(G')' = G$. We call G and G' 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 by

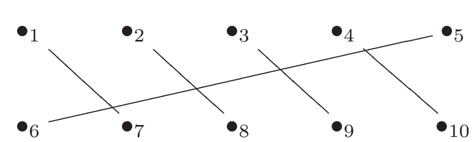


Example 1 establishes that the GTPT of a connected graph need not be connected. Also, it changes the degree sequence of the graph. A relevant question here is whether there exists a graph for which the degree sequence remains invariant under GTPT. Inspired by the degree criteria introduced in [16,39], 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 the GTPT.

Example 2. The following is an example of a degree symmetric graph [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 the PPT criterion 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 the 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 the 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 indicate 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 represent the relative positions of the vertices in the individual layers.

Note that the GTPT keeps a partial symmetric graph unchanged as $A_{i,j} = A_{i,j}^T$ and $D(G) = D(G')$. This leads to the following lemma.

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

The converse of Lemma 1 need not be true. There are many graphs that 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.

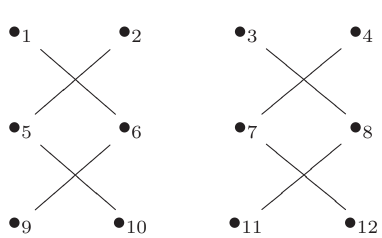
Theorem 2. Let G be a partially symmetric graph with the following properties. (a) Between two vertices of any partition C_i there is no edge: $(v_{i,l},v_{i,k}) \notin E(G)$ for all i,l,k. (b) Either there is no edge between vertices of C_i and C_j or $A_{i,j} = A_{k,l}$ for all $i,j,k,l,i \neq j$ and $k \neq l$. (c) The degrees of all the vertices in a layer are the same, i.e., $d_{C_i}(v_r) = d_{C_i}(v_s)$ for all v_r and $v_s \in C_i$ for all i.

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

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 is not necessary. There are classes of partial symmetric graphs generating separable states without satisfying the 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 labeling $\{1,2,\ldots,n\}$. Define $mG = G \cup G \cup \cdots \cup G$ (union of m copies of G) with vertex labeling $\{v_{j,k} : v_{j,k} = jn + k\}$. 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 first 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

$$A(mG) = \text{diag}\{A(G),A(G),\ldots,A(G)(m \text{ times})\} = I_m \otimes A(G),$$

$$D(mG) = \text{diag}\{D(G),D(G),\ldots,D(G)(m \text{ times})\} = I_m \otimes D(G),$$

$$L(mG) = \text{diag}\{L(G),L(G),\ldots,L(G)(m \text{ times})\} = I_m \otimes L(G),$$

$$Q(mG) = \text{diag}\{Q(G),Q(G),\ldots,Q(G)(m \text{ times})\} = I_m \otimes Q(G),$$

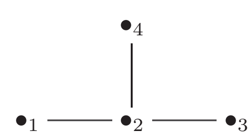
where I_m denotes the identity matrix of order m. Trivially, $\rho_l(mG) = \frac{L(mG)}{\text{tr}[L(mG)]}$ and $\rho_q(mG) = \frac{Q(mG)}{\text{tr}[Q(mG)]}$ are separable states. This result may be expressed as follows.

Lemma 2. For any graph G, $\rho_l(mG)$ and $\rho_q(mG)$ represent separable bipartite states of dimension $m \times n$ with respect to standard labeling on mG.

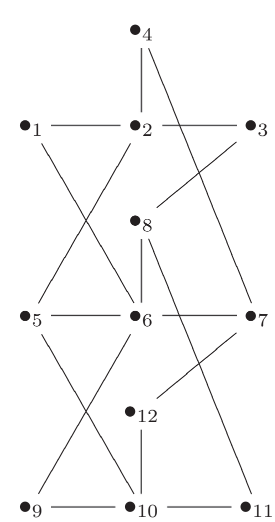
Note that G may not correspond to a separable state but mG always represents a separable state. This lemma is significant as it suggests more general conditions for separability.

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

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



In addition, H is a graph given in Example 3. Then the graph $G \bowtie H$ is



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

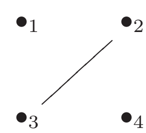
$$\rho(d, p_{\text{sym}}) = p_{\text{sym}} \frac{2}{d^2 + d} P_{\text{sym}} + (1 - p_{\text{sym}}) \frac{2}{d^2 - d} P_{\text{as}},$$

where $P_{\text{sym}} = \frac{1}{2}(1 + P)$ and $P_{\text{as}} = \frac{1}{2}(1 - P)$ 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

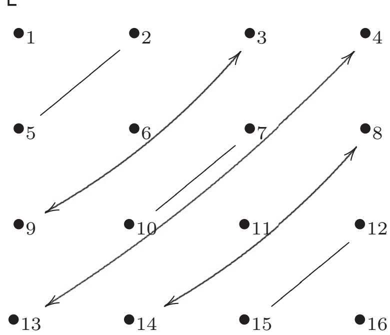
$$\rho(2,0) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.5 & -0.5 & 0 \\ 0 & -0.5 & 0.5 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$\equiv$



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

$\equiv$



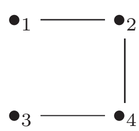
It is easy to verify that these graphs are not degree symmetric and hence not partially symmetric. Further, these graphs represent entangled states.

III. NONLOCAL QUANTUM OPERATION ON GRAPHS

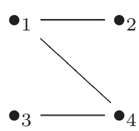
Observe that the definition of partially symmetric graphs relies on the labeling of the vertices. In fact, in the graph-theoretic approach of interpretation of quantum states, it is well known that properties of a density matrix derived from a graph are vertex labeling contingent. A graph that represents a separable state corresponding to a vertex label may also produce an entangled state for a different vertex label. In this section we describe graph isomorphism as a nonlocal 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 labeled vertices given below represents a separable state:

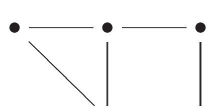


whereas $\rho_l(G_2)$ represents an entangled state for the following graph G_2 with different vertex labeling:



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 labeling and the states $\rho_l(G)$ corresponding to a star graph with respect to any labeling are entangled [16]. In [16] it was also asked if there exist any other graphs that 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 labeling, the graph represents an entangled state. In fact, this graph has no vertex labeling for which it can be made a partially symmetric graph.

Example 7. The graph G for which no vertex labeling produces a partially symmetric graph is



(3)

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

(i) *E graph.* Independent of vertex labeling, all quantum states related to this graph are entangled.

(ii) *S graph.* Independent of vertex labeling, all quantum states related to this graph are separable.

(iii) *ES graph.* Quantum states related to some of the vertex labeling are entangled and others are separable.

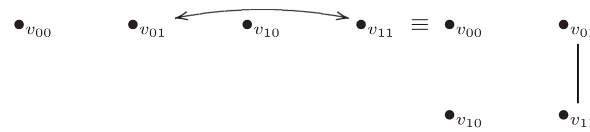
Obviously the completely connected graph is an S graph, the star graph is an E graph, and the graph in Example 7 is an E graph.

In this section, we are interested in ES graphs. These graphs provide a platform for generating entanglement using graph isomorphism as a nonlocal operation. Changing the vertex labeling on a graph representing a separable state generates its isomorphic copy representing an entangled state. It was 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 $\phi : V(G_1) \rightarrow V(G_2)$ defined as

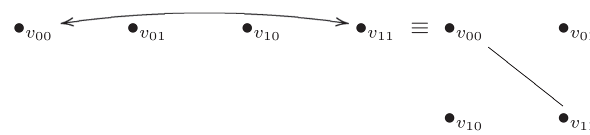
$$\phi(1) = 2, \quad \phi(2) = 1, \quad \phi(3) = 3, \quad \phi(4) = 4$$

act as a mixed state entanglement generator in Example 6. The following example of a 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 $\frac{1}{\sqrt{2}}\,|0+1\rangle\,|1\rangle$:

$G_1 =$ 

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

$G_2 =$ 

The 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 ϕ 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 rest of this work we try to address this question.

Definition 4. In a graph G the partial degree of a vertex $v_{i,k} \in C_i$, with respect to 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 with respect to layer C_j if $(v_{i,k},v_{j,l})$ and $(v_{i,l},v_{j,k}) \in E(G)$.

Here $ld_{C_j}(v_{i,k})$ is the number of vertices internally related to $v_{i,k}$ in C_i with respect to C_j for a partial symmetric graph.

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

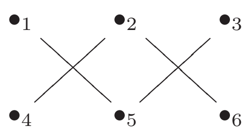
The incidence set of $v \in V(G)$ is $I_G(v) = \{w : (w,v) \in E(G)\}$, that is, a set of all vertices incident to vertex v. The incidence interchange between two vertices u,v, denoted by $u \overset{i}{\leftrightarrow} v$, is a graphical operation to construct a graph H from G, defined as

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

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 preexisting particles, but a purely mathematical operation between two formal particles induced by how we bipartition the graph. Hence there is no contradiction with the physical principle of the nonincrease of entanglement under LOCC. 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.

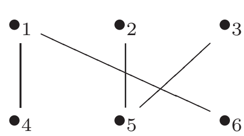
Note that H is a layered graph and is also isomorphic to G. Let us see an example.

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)

Here 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. Also, $dl_{C_1}(1) = 1$ but $dl_{C_1}(2) = 2$. After interchanging the vertex labels of 1 and 2 the new graph is H, which is partially asymmetric. It can be generalized for an arbitrary partially symmetric graph.

If we let in a partially symmetric graph G, $ld_{C_j}(v_{i,k}) \geqslant ld_{C_j}(v_{i,l})$, then $ld_{C_j}(v_{i,k}) - ld_{C_j}(v_{i,l}) \geqslant 1$. Here $ld_{C_j}(v_{i,k})$ and $ld_{C_j}(v_{i,l})$ represent the number of internally related vertices in C_i of $v_{i,k}$ and $v_{i,l}$ with respect to 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 labels there will be at least one edge incident to $v_{i,s}$ without any complement as the complement edge is misplaced by the interchange. Hence, the new graph H, isomorphic to G, is partially asymmetric. This can be expressed as a lemma.

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

Also, $(v_{i,s},v_{j,l}) \notin E(G)$ implies the 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 $(v_{i,l},v_{j,k}) \in E(G)$ ($i \neq j$ and $l \neq k$), but $(v_{i,s},v_{j,l}) \notin E(G)$ for some s, where G is a partially symmetric graph. The interchange of the vertex labels of $v_{i,s}$ and $v_{i,l}$ will generate the partial asymmetric graph H.

This exchange of labels may not generate partial asymmetry in all the cases. Suppose that any two vertices of C_i are not internally related with respect to C_j. Hence, any edge between vertices of C_i and C_j is of the form $(v_{i,k},v_{j,k}) \forall k = 1,2,\ldots,n$. Consider any two vertices of C_i, say, $v_{i,l}$ and $v_{i,k}$. The interchange of the vertex labels 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 write it as a lemma.

Lemma 8. Suppose any two vertices of C_i are not internally related with respect to C_j. Also assume that $ld_{C_j}(v_{i,l}) = ld_{C_j}(v_{i,k}) \forall k,l = 1,2,\ldots n$. Then the interchange of the vertex labels of any two vertices of C_i will not generate partial asymmetry.

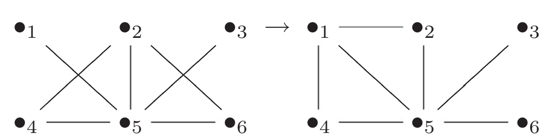
Graph isomorphism is an equivalence relation on the set of all simple graphs, which forms disjoint equivalence classes. Let $\mathcal{G}$ be one such class and $\mathcal{L}$ be the set of all isomorphisms on $\mathcal{G}$. Here $\circ$ is the composition of mappings.

Trivially $(\mathcal{L},\circ)$ forms a group that is a permutation group over $\#[V(G)]$ elements. For an ES graph $\mathcal{G} = \mathcal{E} \cup \mathcal{S}, \mathcal{E} \cap \mathcal{S} = \phi$, $\mathcal{E} \neq \phi$, and $\mathcal{S} \neq \phi$. Here $\mathcal{E}$ 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 that 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 of generating a mixed entangled state from a mixed separable state. Consider two isomorphic graphs



The 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 are separable but for the second graph ρ_l and ρ_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 generalized these results to $m\times n$ systems.

In another direction, our work proposes the use 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 such as LOCC, 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 puts forth a number of problems or directions for future investigation. (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 the combinatorial formulation of separable states? (c) Can the bipartite separability criterion arising from partially symmetric graphs be generalized 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 contributes to the graphical representation of quantum mechanics, in general, and the separability problem, in particular.

ACKNOWLEDGMENTS

This work was partially supported by the project "Graph theoretical aspects in quantum information processing" [Grant No. 25(0210)/13/EMR-II] funded by Council of Scientific and Industrial Research, New Delhi. S.D. is grateful to the Ministry of Human Resource Development, Government of the Republic of India, for a doctoral fellowship. We would like to thank the anonymous referee for constructive comments.

APPENDIX

The following is a proof of Theorem 1.

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

$$\rho_l(G) = \sum_i p_i \rho_i^A \otimes \rho_i^B$$

$$\begin{aligned}
\Rightarrow \rho_l(G)^{T_B} &= \sum_i p_i \rho_i^A \otimes \left(\rho_i^B\right)^{T_B} \\
&= \frac{1}{\mathrm{Tr}[L(G)]}[L(G)]^{T_B} \\
&= \frac{1}{\mathrm{Tr}[L(G)]}\{[D(G)]^{T_B} - [A(G)]^{T_B}\} \\
&= \frac{1}{\mathrm{Tr}[L(G)]}[D(G) - A(G')] \\
&= \frac{1}{\mathrm{Tr}[L(G)]}[D(G) - D(G') + D(G') - A(G')] \\
&= \frac{1}{\mathrm{Tr}[L(G)]}[D(G) - D(G') + L(G')] \\
&= \frac{1}{\mathrm{Tr}[L(G')]}L(G') + \frac{1}{\mathrm{Tr}[L(G)]}[D(G) - D(G')] \\
&\quad \times \{\because d(G)=d(G')\Rightarrow \mathrm{Tr}[L(G)] = \mathrm{Tr}[L(G')]\},
\end{aligned}$$

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

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

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

The following is a 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 normalized eigenvectors, $u_r u_r^t$ is a trace 1 positive-semidefinite matrix for each r. Since there are no edges between any two vertices n of any layer C_i, $A_i = 0$ for all i. Further, $D_i = \mathrm{diag}\{d_i\} = d_i I$ since $A_{i,j} = A_{k,l}$ for all $i,j,k,l, i \neq j$ and $k \neq l$. Then

$$L(G) = \begin{bmatrix} d_0.I & A_{0,1} & A_{0,2} & \cdots & A_{0,(m-1)} \\ A_{0,1} & d_1.I & A_{0,2} & \cdots & A_{0,(m-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{0,(m-1)} & A_{1,(m-1)} & A_{2,(m-1)} & \cdots & d_{m-1}.I \end{bmatrix}$$

$$= \begin{bmatrix} d_0 \sum_r u_r u_r^t & \sum_r \lambda_r u_r u_r^t & \sum_r \lambda_r u_r u_r^t & \cdots & \sum_r \lambda_r u_r u_r^t \\ \sum_r \lambda_r u_r u_r^t & d_1 \sum_r u_r u_r^t & \sum_r \lambda_r u_r u_r^t & \cdots & \sum_r \lambda_r u_r u_r^t \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_r \lambda_r u_r u_r^t & \sum_r \lambda_r u_r u_r^t & \sum_r \lambda_r u_r u_r^t & \cdots & d_{(m-1)} \sum_r u_r u_r^t \end{bmatrix}$$

$$= \sum_r \begin{bmatrix} d_0 & \lambda_r & \lambda_r & \cdots & \lambda_r \\ \lambda_r & d_1 & \lambda_r & \cdots & \lambda_r \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \lambda_r & \lambda_r & \lambda_r & \cdots & d_{m-1} \end{bmatrix} \otimes u_r u_r^t$$

$$= \sum_r B(r) \otimes u_r u_r^t,$$

where

$$B(r) = \begin{bmatrix} d_0 & \lambda_r & \lambda_r & \cdots & \lambda_r \\ \lambda_r & d_1 & \lambda_r & \cdots & \lambda_r \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \lambda_r & \lambda_r & \lambda_r & \cdots & d_m \end{bmatrix}.$$

Note that $A_{i,j} = 0 \Rightarrow b_{i,j} = 0$. Now we want to show that B is a positive-semidefinite matrix.

Note that the spectral radius of $A_{i,j} \leqslant \|A_{i,j}\|_\infty$, where $\|A_{i,j}\|_\infty$ is the subordinate matrix norm defined by $\|A_{i,j}\|_\infty = \max_i \sum_{j=1}^n |a_{i,j}|$. In addition, $d_i = \sum_{k=0}^{m-1} \max_i \sum_{j=1}^n |a_{i,j}| = m \max_i \sum_{j=1}^n |a_{i,j}|$. Then $(m-1)\lambda_r \leqslant (m-1) \times$ (spectral radius of $A_{i,j}$) $\leqslant d_i \forall i$. 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. The result follows similarly for $\rho_q(G)$. ■

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