Quantum Information Processing (2022) 21:152
https://doi.org/10.1007/s11128-022-03483-z

Entanglement and separability of graph Laplacian quantum states

Anoopa Joshi[1] · Parvinder Singh[2] · Atul Kumar[1]

Received: 18 October 2021 / Accepted: 7 March 2022 / Published online: 7 April 2022

Abstract
In this article, we study the entanglement properties of multi-qubit quantum states using a graph-theoretic approach. For this, we define entanglement and separability for m-qubit quantum states associated with a weighted graph on 2^m vertices. We further explore the properties of a block graph and a star graph to demonstrate criteria for entanglement and separability of these graphs.

Keywords Graph Laplacian operators · Density operators · Quantum entanglement · Block graphs · Star graphs

List of symbols

1. $||x||$ Absolute value of $x=(\sqrt{x\bar{x}})$.
2. $\mathrm{Tr}(A)$ Trace of a matrix A.
2. $\det(A)$ Determinant of a matrix A.
4. $D(G)$ The degree matrix of (G, a).
5. ${\rho_G}^{PT}$ Partial transpose of the density operator of a graph G.
6. $\bar{\rho_G}^{PT}$ Conjugate partial transpose of the density operator of a graph G.
7. A^* Conjugate transpose of A.
8. $|E(G)|$ Number of edges in G.

1 Introduction

Quantum information and computation has emerged as an interdisciplinary research platform offering several potential applications in diverse academic domains. The efficient advantages offered by quantum resources are due to entanglement and nonlocal

✉ Atul Kumar
atulk@iitj.ac.in

[1] Indian Institute of Technology Jodhpur, Jodhpur, Rajasthan, India

[2] Central University of Punjab, Bathinda, India

correlations existing between qubits as identified by entanglement measures, Bell-type inequalities and quantum discord. Recent trends in quantum information and computation have shown that applications of entanglement and nonlocality are being recognized in computing, security, machine learning, deep learning, biology, computational chemistry, finance and image processing. With the ever-growing applications of entanglement, there is also a need to classify and quantify entanglement and correlations in multiqubit networks. For example, the entanglement versus separability problem for two-qubit pure and mixed states are well established but the classification and quantification of entanglement in multi-particle systems [2, 18, 31, 34, 35] are increasingly complicated and hence require a much better physical interpretation and understanding. For a three-qubit pure state, several effective criteria have been defined, e.g., the entanglement criterion for states belonging to classes of three qubit pure states has been achieved by a complete stochastic local operations and classical communication (SLOCC) characterization [7, 9, 21]. Considering a multiuser network, classifying entanglement in multi-qubit systems is an important problem and has a special attribute in quantum theory [12, 17, 18]. However, with the increase in number of qubits the complexity increases enormously and proposing a general description to address entanglement versus separability becomes very challenging even for multi-qubit pure states. Clearly, the analysis of multi-qubit mixed states is even more intricate and demanding.

The graph-theoretic approaches are quite handy to solve numerous research problems [32, 33]. In one of its efficient approaches, the graph-theoretical approach has shown its outstanding potential toward quantum physics [13, 18] and information theory [3, 6, 8]. For this, the pictorial representation and physical interpretation of quantum states are provided by graphs [1, 5, 15]. The theory has been further used to model unitary operations and to interpret entanglement or separability properties of quantum states [4, 5, 10, 11, 15]. One of the important ways to define quantum states and their properties is to use the concept of density operators which can be further characterized by normalized Laplacian matrices for graphs [14, 26]. Likewise, we can relate any graph, to a particular quantum state by using its density operator. In particular, quantum states of simple and weighted graphs have been introduced in [5] and [15], respectively, where density operators are normalized combinatorial Laplacians having a unit trace. Moreover, a density operator—acting on a Hilbert space $\mathbb{R}^{n\times n}$ or $\mathbb{C}^{n\times n}$ with respect to the weights of edges of a graph—carries a block structure which can be associated with subsystems. In addition, an m-partite density operator acts on a Hilbert space $\mathbb{R}^{q_1}\otimes\mathbb{R}^{q_2}\otimes\ldots\otimes\mathbb{R}^{q_m}$ or $\mathbb{C}^{q_1}\otimes\mathbb{C}^{q_2}\otimes\ldots\otimes\mathbb{C}^{q_m}$, where $\otimes$ represents a tensor product [15, 16].

In this article, we readdress entanglement versus separability problem using the graph-theoretic approach for multi-qubit systems. For this, we explore graph-theoretical interpretations of entanglement and separability for n-qubit states associated with weighted, block and star graphs. We start our discussion with demonstrating a condition for the Laplacian of a weighted graph to be positive semi-definite and then use this condition to introduce the notion of a density operator for a multi-qubit graph/state. We further propose conditions for a density operator of a weighted graph to represent a pure or a mixed state. In addition, we also analyze entanglement and separability of states associated with weighted graphs to demonstrate many interesting conditions to characterize entanglement properties of weighted graphs. We further study entanglement properties of block graphs and star graphs. Our analysis shows that the state associated with a weighted graph (G, a) is entangled if at least one of the blocks of graph is associated with an entangled state. Moreover, if every vertex of a n-qubit graph G has degree $k \geq 2$ such that G has no cut-vertex, then the graph G is associated with a separable state. Interestingly, our results demonstrate that if r vertices are deleted from a star graph on 2^m vertices then the resulting graph on 2^s vertices is associated with an entangled quantum state such that $0 \leq r \leq 2(2^{(m-1)} - 1)$. We further analyze the degree of entanglement in a star graph G' obtained by adding adjacent edges to the original graph G, and show that the resultant graph G' will have at least one block which is associated with an entangled state such that the entanglement measure of blocks of G' would not exceed the entangled measure of blocks of G.

The article is organized as follows: In Sect. 2, we briefly discuss the properties of weighted graphs, the associated Laplacian operators and partial transpose of weighted graphs. In Sect. 3, we propose a condition for the Laplacian of a weighted graph (G, a) on $n = 2^m$ vertices to be positive semi-definite and address entanglement and separability issues in multi-qubit weighted graphs. Section 4 is dedicated toward characterizing entanglement properties of weighted, block and start graphs. In this section, we demonstrate several effective criteria to study the separability of n-qubit entangled states. Finally, in Sect. 5, we conclude the article.

2 Preliminaries

In this section, we first provide a brief review of weighted graphs and important terminologies such as adjacency matrix, degree matrix and Laplacian matrix which we will be using in the upcoming sections of the article to represent quantum states associated with a given weighted graph.

2.1 Weighted graphs

A *graph* G on n vertices is a pair $(V(G), E(G))$, where $V(G) = \{v_1, v_2, \ldots, v_n\}$ is the set of vertices, and $E(G) \subseteq V(G) \times V(G)$ is the set of edges. Similarly, a *weighted graph* (G, a) is a graph together with a weight function $a : E(G) \rightarrow \mathbb{F}$ defined as follows: let $v_i, v_j \in V(G)$, and $(v_i, v_j) \in E(G)$, then $a(v_i, v_j)$ is weight from v_i to v_j, $1 \leq i, j \leq n$. If two distinct vertices v_i and v_j are connected with an edge, then we denote it by $v_i \sim v_j$. Clearly, $v_i = v_j$; $(v_i, v_i) \in E(G)$, is a self-loop at vertex v_i having the weight $a(v_i, v_i)$. In the special case when all nonzero weights in (G, a) are equal to 1, and there are no self-loops, it is called a *simple graph*. Further, if (G, a) is a weighted graph on n vertices then the *adjacency matrix* of (G, a), denoted by $A(G)$, is a $n \times n$ matrix with (i, j)-th entry equals $a_{ij} = a(v_i, v_j)$ if $v_i \sim v_j$, otherwise 0.

2.1.1 Laplacian matrix of a weighted graph on $\mathbb{R}$

A weighted graph (G, a) is a graph together with a weight function $a : E(G) \rightarrow \mathbb{R}$ defined as follows,

1. $a(v_i, v_j) \neq 0$ if $v_i, v_j \in E(G)$ and 0 otherwise.
2. $a(v_i, v_j) = a(v_j, v_i)$

We can now proceed to define the *Laplacian matrix* of a weighted graph G as [15, 20]

$$L(G) = D(G) - A(G) + D_0(G), \tag{1}$$

where $D_0(G)$ is a diagonal matrix with i-th diagonal entry equals to $a(v_i, v_i)$ and $D(G)$ is the *degree matrix* of (G, a). The degree matrix is a diagonal matrix with the i-th diagonal entry equals to the sum of all entries of i-th row (or column) of $A(G)$, i.e., $\sum_{j=1}^{n} a_{ij}$. For a simple graph, the degree matrix $D(G)$ of a vertex $v_i \in V(G)$ is defined as the number of edges in $E(G)$ incident on v_i.

2.1.2 Laplacian matrix of a weighted graph on $\mathbb{C}$

One can further define a weighted graph (G, a) with a weight function $a : E(G) \rightarrow \mathbb{C}$ as,

1. $a(v_i, v_j) \neq 0$ if $v_i, v_j \in E(G)$ and 0 otherwise.
2. $a(v_i, v_j) = \overline{a(v_j, v_i)}$

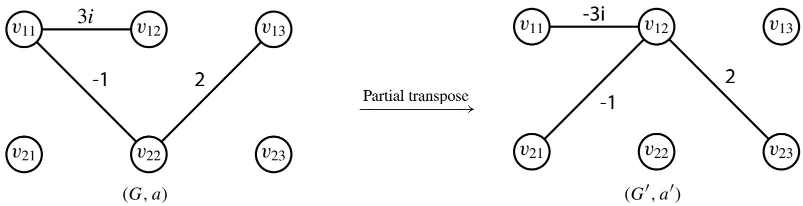
The generalized Laplacian of a graph (G, a), which includes loops, is $L(G) = D(G) + A(G) - D_0(G)$ [15] where the degree matrix with i-th diagonal entry of vertex v_i is given by [15]

$$d_{v_i v_i} = \sum_{v_i \in V(G), v_i \neq v_j} ||a(v_i, v_j)|| + a(v_i, v_i).$$

In general, $L(G)$ is not positive semi-definite, however, for a simple graph it is positive semi-definite. For simple graphs, $D_0(G) = 0$ and $L(G) = D_1(G) + D_2(G) - A_1(G) - A_2(G)$, where $D_1(G)$ and $D_2(G)$ are diagonal matrices, and diagonal entries are row sum of $A_1(G)$ and $A_2(G)$, respectively. Therefore, the Laplacian of a simple graph can be re-expressed as sum of Laplacian matrices of simple graphs. We utilize this property to analyze separability and entanglement problems in star graphs. In order to facilitate the discussion of our results, we also briefly discuss the decomposition of a Laplacian matrix for simple graphs in the Appendix.

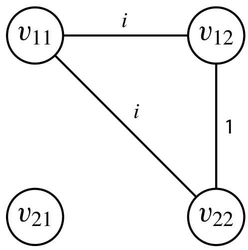
2.2 Conjugate partial transpose of a weighted graph

Let (G, a) be a graph on $n = pq$ vertices and vertex set $V(G) = \{v_{ij} | i = 1, 2, \ldots p$ and $j = 1, 2, \ldots q\}$. Using (G, a), if one draws edges of the form (v_{il}, v_{kj}), in place of all edges of the form (v_{ij}, v_{kl}) where the weight is $\overline{a(v_{ij}, v_{kl})}$, for all $j \neq l$ then the resulting graph (G', a') is called as the conjugate partial transpose of the original graph (G, a) [11, 15, 19]. For example,



It is important to note that for a graph (G, a), the conjugate partial transpose of the Laplacian matrix $L(G)$ may or may not be equal to the Laplacian matrix of the conjugate partial transpose of (G, a). For example,

Example 1 Consider the following graph G_1.



G_1

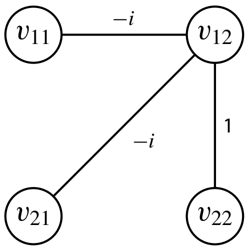
Clearly, the Laplacian matrix of G_1 is

$$L(G_1) = \begin{bmatrix} 2 & i & 0 & i \\ -i & 2 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ -i & 1 & 0 & 2 \end{bmatrix},$$

and the conjugate partial transpose of $L(G_1)$ is

$$L(\bar{G}_1)^{PT} = \begin{bmatrix} 2 & i & 0 & 0 \\ -i & 2 & -i & 1 \\ 0 & i & 0 & 0 \\ 0 & 1 & 0 & 2 \end{bmatrix}.$$

Whereas, the conjugate partial transpose of the graph G_1, i.e., $G_1{}'$ is



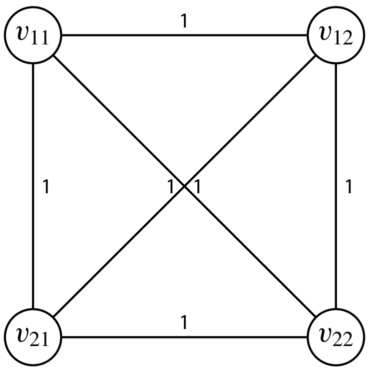
$G_1{}'$

and the Laplacian matrix of $G_1{}'$ is

$$L(G_1{}') = \begin{bmatrix} 1 & -i & 0 & 0 \\ i & 3 & -i & 1 \\ 0 & i & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

Therefore, $L(G_1{}') \neq L(\bar{G}_1)^{PT}$.

Example 2 Consider the following graph G_2.



G_2

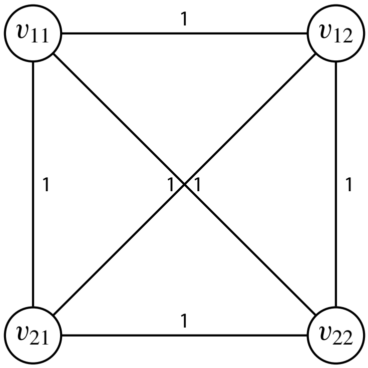
The Laplacian matrix of G_2 is

$$L(G_2) = \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix},$$

and the partial transpose of $L(G_2)$ is

$$L(G_2)^{PT} = \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix}.$$

Similarly, the partial transpose of the graph G_2 is



$G_2{}'$

and the Laplacian matrix of $G_2{}'$ is

$$L(G_2{}') = \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix}$$

Here, $L(G_2{}') = L(G_2)^{PT}$.

3 Density operator of a graph

In general, the state of a quantum system may not be in a pure state. Due to the inherent statistical nature of quantum theory, the description of a quantum state using density operator formalism provides a much better physical interpretation of the system under study. The density operator formalism is also considered as an alternate representation for pure states, and finds its applications in quantum error correction, quantum noise, quantum communication and measures of quantum entanglement [25, 34]. For studying several interesting properties of entanglement and nonlocality, the concepts of density operator, reduced density operator and partial transpose are widely utilized [1, 5, 11, 15, 19] . Here, we propose a graph-theoretic study using a density operator mechanism to understand entanglement and separability in multiqubit pure states.

For this, we first define the density operator ρ_G of a graph (G, a) considering the case where the Laplacian of the graph is a positive semi-definite matrix and is given by the following expression

$$\rho_G = \frac{1}{Tr(L(G))} L(G)$$

We now proceed to demonstrate a necessary and sufficient condition for the Laplacian matrix of a graph to be positive semi-definite. For a graph G associated with an m-qubit state, vertices are column basis on $\mathbb{R}^{q_1} \otimes \mathbb{R}^{q_2} \otimes \ldots \otimes \mathbb{R}^{q_m}$ or $\mathbb{C}^{q_1} \otimes \mathbb{C}^{q_2} \otimes \ldots \otimes \mathbb{C}^{q_m}$.

Theorem 3.1 *Let (G, a) be a weighted graph on n vertices. If the Laplacian matrix $L(G) = [l_{ij}]_{n \times n}$ is positive semi-definite then $l_{ii} \geq 0$ and det $\begin{bmatrix} l_{ii} & l_{ij} \\ l_{ji} & l_{jj} \end{bmatrix} \geq 0$ for all i, j.*

Proof $L(G)$ is positive semi-definite if $x^* L(G) x \geq 0$ for any vector $x = [x_1, x_2, \ldots, x_n]^T \in \mathbb{C}^n$, where $x^* = [\bar{x_1}, \bar{x_2}, \ldots, \bar{x_n}]$ is conjugate transpose of x, i.e.,

$$\begin{bmatrix} \bar{x_1} & \bar{x_2} & \ldots & \bar{x_n} \end{bmatrix} \begin{bmatrix} l_{11} & l_{12} & \ldots & l_{1n} \\ l_{21} & l_{22} & \ldots & l_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ l_{n1} & l_{n2} & \ldots & l_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \geq 0,$$

or

$$\bar{x_1}(l_{11}x_1 + l_{12}x_2 + \cdots + l_{1n}x_n) + \cdots + \bar{x_n}(l_{n1}x_1 + l_{n2}x_2 + \cdots + l_{nn}x_n) \geq 0,$$

or

$$\begin{aligned} &\bar{x_1}(l_{11}x_1 + l_{12}x_2 + \cdots + l_{1n}x_n) + \cdots + \bar{x_n}(l_{n1}x_1 + l_{n2}x_2 + \cdots \\ &\quad + l_{nn}x_n) + (n-2)(l_{11}\bar{x_1}x_1 + l_{22}\bar{x_2}x_2 + \cdots + l_{nn}\bar{x_n}x_n) \\ &\quad - (n-2)(l_{11}\bar{x_1}x_1 + l_{22}\bar{x_2}x_2 + \cdots + l_{nn}\bar{x_n}x_n) \geq 0, \end{aligned}$$

or

$$\begin{aligned} &\{\bar{x_1}(l_{11}x_1 + l_{12}x_2) + \bar{x_2}(l_{21}x_1 + l_{22}x_2)\} + \cdots + \{\bar{x_{n-1}}(l_{n-1n-1}x_{n-1} \\ &\quad + l_{n-1n}x_n) + \bar{x_n}(l_{nn-1}x_{n-1} + l_{nn}x_n)\} \\ &\geq (n-2)(l_{11}\bar{x_1}x_1 + l_{22}\bar{x_2}x_2 + \cdots + l_{nn}\bar{x_n}x_n), \end{aligned}$$

which implies

$$\begin{bmatrix}\bar{x_1} & \bar{x_2}\end{bmatrix}\begin{bmatrix}l_{11} & l_{12}\\ l_{21} & l_{22}\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix} + \cdots + \begin{bmatrix}\bar{x_{n-1}} & \bar{x_n}\end{bmatrix}\begin{bmatrix}l_{n-1n-1} & l_{n-1n}\\ l_{nn-1} & l_{nn}\end{bmatrix}\begin{bmatrix}x_{n-1}\\ x_n\end{bmatrix} \geq 0.$$

Thus, we have

$$\begin{bmatrix}\bar{x_i} & \bar{x_j}\end{bmatrix}\begin{bmatrix}l_{ii} & l_{ij}\\ l_{ji} & l_{jj}\end{bmatrix}\begin{bmatrix}x_i\\ x_j\end{bmatrix} \geq 0 \text{ for all } i < j.$$

Therefore, $l_{ii} \geq 0$ and $det\left(\begin{bmatrix}l_{ii} & l_{ij}\\ l_{ji} & l_{jj}\end{bmatrix}\right) \geq 0$ for all i, j. □

Theorem 3.2 *Let (G, a) be a weighted graph on $n = 2^m$ vertices associated with an m-qubit state, and $\rho_G = [\rho_{ij}]_{n\times n}$ be its density operator. If (G, a) represents a pure state, then $\sum_{i=1}^{n-1}\sum_{j>i}^{n} \rho_{ii}\rho_{jj} = \sum_{i<j} ||\rho_{ij}||^2$.*

Proof If ρ_G is a pure state, then $\mathrm{Tr}({\rho_G}^2) = 1$, i.e.,

$${\rho_{11}}^2 + {\rho_{22}}^2 + \cdots + {\rho_{nn}}^2 + 2(||\rho_{12}||^2 + \cdots + ||\rho_{1n}||^2 + \cdots + ||\rho_{n-1n}||^2) = 1,$$

which implies that,

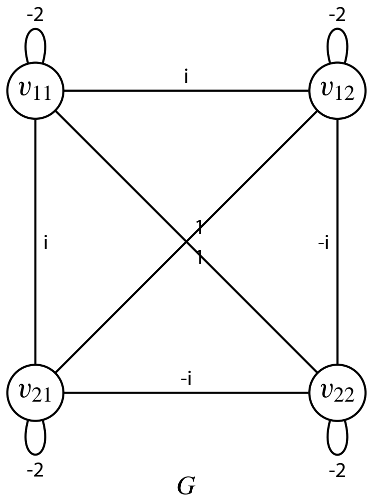
$$\begin{aligned}&\rho_{11}\rho_{22} + \cdots + \rho_{11}\rho_{nn} + \cdots + \rho_{n-1n-1}\rho_{nn}\\ &\quad = ||\rho_{12}||^2 + \cdots + ||\rho_{1n}||^2 + \cdots + ||\rho_{n-1n}||^2.\end{aligned}$$

Hence,

$$\sum_{i=1}^{n-1}\sum_{i<j}^{n} \rho_{ii}\rho_{jj} = \sum_{i<j} ||\rho_{ij}||^2.$$

□

Example 3 The following graph is associated with a pure state as $\mathrm{Tr}({\rho_G}^2) = 1$, and $\rho_{11}(\rho_{22} + \rho_{33} + \rho_{44}) + \rho_{22}(\rho_{33} + \rho_{44}) + \rho_{33}\rho_{44} = ||\rho_{12}||^2 + ||\rho_{13}||^2 + ||\rho_{14}||^2 + ||\rho_{23}||^2 + ||\rho_{24}||^2 + ||\rho_{34}||^2 = 6$.



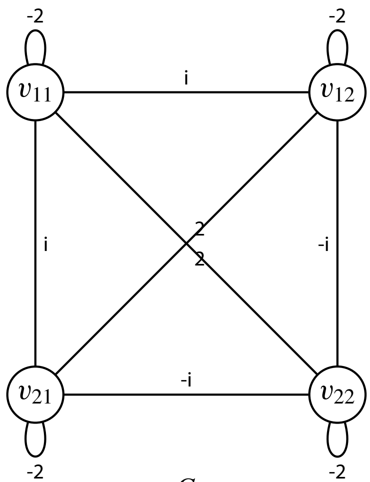
G

$$\rho_G = \frac{1}{4}\begin{bmatrix} 1 & i & i & 1 \\ -i & 1 & 1 & -i \\ -i & 1 & 1 & -i \\ 1 & i & i & 1 \end{bmatrix}$$

If (G, a) represents a mixed state, then $\text{Tr}({\rho_G}^2) < 1$, so the following result holds,

Corollary 3.3 *Let (G, a) be a weighted graph on $n = 2^m$ vertices associated with an m-qubit state, and $\rho_G = [\rho_{ij}]_{n\times n}$ be its density operator. If (G, a) represents a mixed state, then $\sum_{i<j} ||\rho_{ij}||^2 < \sum_{i=1}^{n-1}\sum_{j>i}^{n} \rho_{ii}\rho_{jj}$.*

Example 4 The following graph is associated with a mixed state as $\text{Tr}({\rho_G}^2) < 1$, and $\rho_{11}(\rho_{22} + \rho_{33} + \rho_{44}) + \rho_{22}(\rho_{33} + \rho_{44}) + \rho_{33}\rho_{44} > ||\rho_{12}||^2 + ||\rho_{13}||^2 + ||\rho_{14}||^2 + ||\rho_{23}||^2 + ||\rho_{24}||^2 + ||\rho_{34}||^2$.



G

$$\rho_G = \frac{1}{8}\begin{bmatrix} 2 & i & i & 2 \\ -i & 2 & 2 & -i \\ -i & 2 & 2 & -i \\ 2 & i & i & 2 \end{bmatrix}$$

Theorem 3.4 *Let (G, a) be a weighted graph on $n = 2^{p+q}$ vertices, where q is prime and the associated density operator ρ_G is a block matrix of order 2^q consisting of blocks of order 2^p. Then, $a(v_{ij}, v_{kl}) = \overline{a(v_{il}, v_{kj})}$ and $a(v_{ij}, v_{kl}) \in \mathbb{R}$ for $j = l$ if and only if $\bar{\rho_G}^{PT} = \rho_G = \rho_{G'}$ where $\rho_{G'}$ is a density operator of conjugate partial transpose of the graph (G, a).*

Proof Let $a(v_{ij}, v_{kl})$ is a weight from vertex v_{ij} to v_{kl}.
Moreover, we have

$$\rho_G = \frac{1}{Tr(L(G))} L(G) = \frac{1}{Tr(L(G))} \begin{bmatrix} l_{11} & l_{12} & \dots & l_{12^n} \\ l_{21} & l_{22} & \dots & l_{22^n} \\ . & . & \dots & . \\ . & . & \dots & . \\ . & . & \dots & . \\ l_{2^n1} & l_{2^n2} & \dots & l_{2^n2^n} \end{bmatrix},$$

where,

$$L(G) = \begin{bmatrix} \begin{bmatrix} l_{11} & \dots & a(v_{11}, v_{12^p}) \\ a(v_{12}, v_{11}) & \dots & a(v_{12}, v_{12^p}) \\ . & \dots & . & . \\ . & \dots & . \\ a(v_{12^p}, v_{11}) & \dots & l_{2^p2^p} \end{bmatrix} & \dots & \begin{bmatrix} a(v_{11}, v_{2^q1}) & \dots & a(v_{11}, v_{2^q2^p}) \\ a(v_{12}, v_{2^q1}) & \dots & a(v_{12}, v_{2^q2^p}) \\ . & \dots & . \\ . & \dots & . \\ a(v_{12^p}, v_{2^q1}) & \dots & a(v_{12^p}, v_{2^q2^p}) \end{bmatrix} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ \begin{bmatrix} a(v_{2^q1}, v_{11}) & \dots & a(v_{2^q1}, v_{12^p}) \\ a(v_{2^q2}, v_{11}) & \dots & a(v_{2^q2}, v_{12^p}) \\ . & \dots & . \\ . & \dots & . \\ a(v_{2^q2^p}, v_{11}) & \dots & a(v_{2^q2^p}, v_{12^p}) \end{bmatrix} & \dots & \begin{bmatrix} l_{rr} & \dots & a(v_{2^q1}, v_{2^q2^p}) \\ a(v_{2^q2}, v_{11}) & \dots & a(v_{2^q2}, v_{2^q2^p}) \\ . & \dots & . \\ . & \dots & . \\ a(v_{2^q2^p}, v_{2^q1}) & \dots & l_{2^n2^n} \end{bmatrix} \end{bmatrix},$$

and $r = (2^q - 1)2^p + 1$. If $a(v_{ij}, v_{kl}) = \overline{a(v_{il}, v_{kj})}$ and $a(v_{ij}, v_{kl}) \in \mathbb{R}$ for $j = l$ then $\bar{L_{ij}}^T = L_{ij} = L(G')_{ij}$ for all i and j, where L_{ij} is ij^{th} block of $L(G)$, and $L(G')$ is the Laplacian matrix of conjugate partial transpose of (G, a). Therefore, $\rho_{G'} = \rho_G = \bar{\rho_G}^{PT}$. The reverse implication is also true. □

4 Entanglement and separability of Weighted graphs

In this section, we discuss the separability and entanglement of weighted graphs on $n = 2^m$ vertices, associated with m-qubit states. We further demonstrate the separability and entanglement of quantum states corresponding to block graphs and star graphs.

It is evident that the density operator ρ_G of a graph (G, a) on $n = pq$ vertices is *separable* if it can be written as a convex combination of the tensor product of density operators ρ_1^i of order p and ρ_2^i of order q, such that [18, 30],

$$\rho_G = \sum_i p_i \rho_1^i \otimes \rho_2^i, \tag{2}$$

where $0 \leq p_i \leq 1$ and $\sum_i p_i = 1$. Moreover, in order to evaluate the degree of entanglement in a two-qubit state, concurrence is considered as one of the standard measures. For example, concurrence of a two-qubit state ρ_G is defined as $C(\rho_G) = max(0, \sqrt{\mu_1} - \sqrt{\mu_2} - \sqrt{\mu_3} - \sqrt{\mu_4})$ [35]. Here $\mu_1 \geq \mu_2 \geq \mu_3 \geq \mu_4$ are eigenvalues of the matrix $\rho_G \tilde{\rho_G}$; $\tilde{\rho_G} = P {\rho_G}^* P$ where asterisk represents complex conjugation and

$$P = \sigma_y \otimes \sigma_y = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}.$$

The value of concurrence $C(\rho_G)$ lies in [0, 1], i.e., if $C(\rho_G) = 0$, then the density operator ρ_G represents a separable state otherwise it is considered as entangled; and if $C(\rho_G) = 1$ then ρ_G represents a maximally entangled state.

Theorem 4.1 *Let (G, a) be a weighted graph on 4 vertices. Suppose the Laplacian $L(G)$ is positive semi-definite having eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$. If $\lambda_1 \leq \lambda_2 + \lambda_3$, then (G, a) is associated with a two-qubit separable state.*

Proof As the Laplacian $L(G)$ is positive semi-definite the density operator $\rho_G = \frac{1}{\mathrm{Tr}(L(G))} L(G)$ is also positive semi-definite. By the definition of $\tilde{\rho_G}$, we have, $\mathrm{Tr}(\rho_G) = \mathrm{Tr}(\tilde{\rho_G}) = 1$ and $\tilde{\rho_G}$ is positive semi-definite. If ρ_G and $\tilde{\rho_G}$ are two positive semi-definite matrices, then the following are equivalent [22, 29, 36]:

1. $\rho_G \tilde{\rho_G}$ is normal, that is, $[\rho_G \tilde{\rho_G}, (\rho_G \tilde{\rho_G})^*] = \rho_G \tilde{\rho_G} (\rho_G \tilde{\rho_G})^* - (\rho_G \tilde{\rho_G})^* \rho_G \tilde{\rho_G} = 0$.
2. $\rho_G \tilde{\rho_G}$ is positive semi-definite.

The eigenvalues of ρ_G are $\frac{\lambda_1}{\sum \lambda_i} \geq \frac{\lambda_2}{\sum \lambda_i} \geq \frac{\lambda_3}{\sum \lambda_i} \geq \frac{\lambda_4}{\sum \lambda_i}$. Let $\nu_1 \geq \nu_2 \geq \nu_3 \geq \nu_4$ be the eigenvalues of $\tilde{\rho_G}$ and $\mu_1 \geq \mu_2 \geq \mu_3 \geq \mu_4$ be the eigenvalues of matrix $\rho_G \tilde{\rho_G}$. Therefore, $\mu_1 \leq \frac{\lambda_1}{\sum \lambda_i} \nu_1 \leq \frac{(\lambda_2 + \lambda_3 + \lambda_4)}{\sum \lambda_i} \nu_1 \leq \mu_2 + \mu_3 + \mu_4$ [29, 37] which implies the concurrence for ρ_G is equal to 0 as $C(\rho_G) = max(0, \sqrt{\mu_1} - \sqrt{\mu_2} - \sqrt{\mu_3} - \sqrt{\mu_4})$. Hence, (G, a) is associated with a separable state. □

Theorem 4.2 *Let (G, a) be a weighted graph on $n = 2^m (m = p + q)$ vertices associated with an m-qubit state. Let $(n - 2)$ vertices are isolated and there is one edge that lies between the remaining two vertices (loops can also be also considered on them). Suppose, $V(G) = \{v_{ij}\}$ is the set of vertices, where $i = 1, 2, \ldots, 2^q$, and $j = 1, 2, \ldots, 2^p$. The graph (G, a) is entangled if and only if the edge lies between v_{ij} and $v_{2^q-(i-1)\ 2^p-(j-1)}$ for any j.*

Proof Let (G, a) be a weighted graph on $n = 2^m(m = p + q)$ vertices associated with an m-qubit state where $(n-2)$ vertices are isolated. If $V(G) = \{v_{ij}\}$ is the set of vertices, where $i = 1, 2, \ldots, 2^q$, and $j = 1, 2, \ldots, 2^p$ then for a two-qubit state, there are four vertices $|00\rangle, |01\rangle, |10\rangle$, and $|11\rangle$. Therefore, a two-qubit quantum state associated with a weighted graph on 4 vertices is entangled if the edge lies between vertices v_{ij} and $v_{2-(i-1)\ 2-(j-1)}$, where $i = 1, 2$ and $j = 1, 2$.

Similarly, for a three-qubit state, there are eight vertices $(|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle)$. Therefore, a quantum state associated with a weighted graph on 8 vertices is entangled if the edge lies between v_{ij} and $v_{2-(i-1)\ 4-(j-1)}$, where $i = 1, 2$ and $j = 1, 2, 3, 4$. Likewise for an m-qubit state, there are 2^m vertices $|\underbrace{000\ldots0}_{m}\rangle, |\underbrace{000\ldots0}_{m-1}1\rangle, \ldots, |0\underbrace{111\ldots1}_{m-1}\rangle, |1\underbrace{000\ldots0}_{m-1}\rangle, \ldots, |\underbrace{111\ldots1}_{m-1}0\rangle$, and $|\underbrace{111\ldots1}_{m}\rangle$ and hence a quantum state associated with a weighted graph on 2^m vertices is entangled if edge lies between v_{ij} and $v_{2^q-(i-1)\ 2^p-(j-1)}$, where $i = 1, 2, \ldots, 2^q$ and $j = 1, 2, \ldots, 2^p$. □

Theorem 4.3 *Let (G, a) be a weighted graph on $n = 2^m$ vertices associated with an m-qubit state. If $det(\rho_G^1) = 0$ then the state associated with (G, a) is separable, where ρ_G^1 is a reduced density operator associated with the first qubit.*

Proof Let $\rho_G = [\rho_{ij}]_{n\times n}$ be a density operator which can be represented as a 2×2 block matrix, i.e.

$$\rho_G = \begin{bmatrix} A & B \\ B^* & C \end{bmatrix}, \tag{3}$$

therefore,

$$\rho_G^1 = \begin{bmatrix} Tr(A) & Tr(B) \\ Tr(B^*) & Tr(C) \end{bmatrix}. \tag{4}$$

Since $det(\rho_G^1) = 0$,

$$\begin{aligned}(\rho_{11} + \cdots + \rho_{\frac{n}{2}\frac{n}{2}})(\rho_{\frac{n}{2}+1\frac{n}{2}+1} + \cdots + \rho_{nn}) \\ - ||(\rho_{1\frac{n}{2}+1} + \rho_{2\frac{n}{2}+2} + \cdots + \rho_{\frac{n}{2}n})||^2 = 0,\end{aligned} \tag{5}$$

or

$$\begin{aligned}(\rho_{11} + \cdots + \rho_{\frac{n}{2}\frac{n}{2}})(\rho_{\frac{n}{2}+1\frac{n}{2}+1} + \cdots + \rho_{nn}) \\ = ||(\rho_{1\frac{n}{2}+1} + \rho_{2\frac{n}{2}+2} + \cdots + \rho_{\frac{n}{2}n})||^2.\end{aligned} \tag{6}$$

From equation (6), if $||\rho_{1\frac{n}{2}+1} + \rho_{2\frac{n}{2}+2} + \cdots + \rho_{\frac{n}{2}n}||^2 = 0$ then either $(\rho_{11} + \cdots + \rho_{\frac{n}{2}\frac{n}{2}}) = 0$ or $(\rho_{\frac{n}{2}+1\frac{n}{2}+1} + \cdots + \rho_{nn}) = 0$. Therefore, either $\rho_G = \begin{bmatrix} A & 0 \\ 0 & 0 \end{bmatrix}$

or $\rho_G = \begin{bmatrix} 0 & 0 \\ 0 & C \end{bmatrix}$ which suggests that ρ_G is separable. On the other hand, if $||\rho_{1\frac{n}{2}+1} + \rho_{2\frac{n}{2}+2} + \cdots + \rho_{\frac{n}{2}n}||^2 \neq 0$, then $\rho_G = \frac{1}{2A}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \otimes A$ or $\rho_G = \frac{1}{2A}\begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix} \otimes A$, hence, ρ_G is separable. □

Theorem 4.4 *Let (G, a) be a weighted graph on $n = 2^m$ vertices associated to an m-qubit state with at least two edges and the density operator ρ_G be a block matrix. If $A_{bc} = A_{cb}{}^*$, where A_{bc} is bc^{th} block of the density operator ρ_G then one cannot identify whether the underlying state is an entangled or a separable state. If $A_{bc} = i^r B_{bc} + i^s C_{bc} + i^t D_{bc}$ for $b < c$, $r = 1$ or 4, $s = 2$ or 3, $t = 1$ or 2 or 3 or 4, where B_{bc} and C_{bc} are positive semi-definite matrices and D_{bc} is a positive semi-definite diagonal matrix such that*

$$E_{bb} = A_{bb} - \sum_{c \neq b}(B_{bc} + C_{bc} + D_{bc}) \geq 0,$$

then the graph G is associated with a separable state.

Proof Let (G, a) be a weighted graph on 2^n $(n = p + q)$ vertices associated with an n-qubit state where the associated density operator ρ_G is a $2^p \times 2^p$ block matrix such that

$$\rho_G = \frac{1}{Tr(L(G))}\begin{bmatrix} A_{11} & A_{12} & \dots & A_{12^p} \\ A_{21} & A_{22} & \dots & A_{22^p} \\ \vdots & \vdots & \vdots & \vdots \\ A_{2^p1} & A_{2^p2} & \dots & A_{2^p2^p} \end{bmatrix}$$

Here, $A_{bc} = A_{cb}{}^*$, so for $b < c$, A_{bc} can be decomposed as $A_{bc} = i^r B_{bc} + i^s C_{bc} + i^t D_{bc}$ where $r = 1$ or 4, $s = 2$ or 3, $t = 1$ or 2 or 3 or 4. Further, B_{bc} and C_{bc} are positive semi-definite matrices and D_{bc} is a positive semi-definite diagonal matrix. Therefore, if $A_{bc} = A_{cb}{}^*$ then $A_{cb} = (-i)^r B_{bc} + (-i)^s C_{bc} + (-i)^t D_{bc}$. Hence, one can evaluate that ρ_G can be written as convex combination of tensor products if $E_{bb} = A_{bb} - \sum_{c \neq b}(B_{bc} + C_{bc} + D_{bc}) \geq 0$. □

Corollary 4.5 *Let $\rho_G = \frac{1}{Tr(L(G))}\begin{bmatrix} A_{11} & A_{12} & \dots & A_{12^p} \\ A_{21} & A_{22} & \dots & A_{22^p} \\ \vdots & \vdots & \vdots & \vdots \\ A_{2^p1} & A_{2^p2} & \dots & A_{2^p2^p} \end{bmatrix}$ be the density operator of a weighted graph (G, a) on $2^{n=p+q}$ vertices where A_{ij} are Hermitian matrices of order 2^q. If $A_{ij} = B_{ij} - C_{ij} + (-1)^m D_{ij}$ for $i \neq j$ where B_{ij} and C_{ij} are positive semi-definite matrices and D_{ij} is a positive semi-definite diagonal matrix such that*

$$A_{ii} - \sum_{j \neq i} A_{ij} \geq 0, \text{ for all } i$$

then the graph G is associated with a separable state where $Tr(L(G)) = \sum_i Tr(E_{ii}) + 2\sum_i \sum_{j>i} Tr(B_{ij}) + Tr(C_{ij}) + Tr(D_{ij})$ *and* $E_{ii} = A_{ii} - \sum_{j \neq i}(B_{ij} + C_{ij} + D_{ij})$.

Corollary 4.6 *Let G be a weighted graph on* $n = 2^m$ $(m \neq 0)$ *vertices associated to an m-qubit state and* ρ_G *be the density operator with* $\rho_G = \bar{\rho_G}^{PT}$. *If all off diagonal blocks are either positive or negative semi-definite and* $A_{ii} \geq \sum_{j \neq i} A_{ij}$, *then the state is associate to a separable state.*

Theorem 4.7 *Let* (G, a) *be a weighted graph on* $n = 2^m$ *vertices associated to an m-qubit state with at least two edges and the density operator* ρ_G *be a block matrix. The state associated with the graph G is entangled if and only if* $A_{ij} \neq {A_{ji}}^*$, *where* A_{ij} *is* ij^{th} *block of* ρ_G; *and* $A_{ij'} \neq {A_{ji'}}^*$ *where* $A_{ij'}$ *is* ij^{th} *block of* $\rho_{G'}$ *where* $\rho_{G'}$ *is a density operator obtained after interchanging columns* C_i *with* C_j, *and corresponding rows* R_i *with* R_j *in* ρ_G.

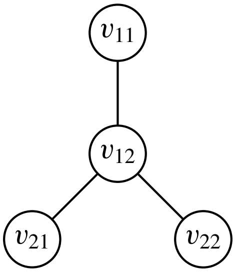
Proof Let (G, a) be a weighted graph on $n = 2^m$ vertices associated to an m-qubit state with at least two edges. The density operator $\rho_G = \frac{1}{Tr(L(G))}\begin{bmatrix} A_{11} & A_{12} & \dots & A_{12^p} \\ A_{21} & A_{22} & \dots & A_{22^p} \\ \vdots & \vdots & \vdots & \vdots \\ A_{2^p1} & A_{2^p2} & \dots & A_{2^p2^p} \end{bmatrix}$ be a block matrix. Let us further assume that $A_{ij} \neq {A_{ji}}^*$, where A_{ij} is ij^{th} block of density operator ρ_G, and $A_{ij'} \neq {A_{ji'}}^*$ where $A_{ij'}$ is ij^{th} block of $\rho_{G'}$.

Clearly, if the density operator ρ_G of a graph (G, a) on $n = 2^m$ vertices is *separable* then it can be written as a convex combination of the tensor product of density operators ρ_1^i and ρ_2^i, such that [18]

$$\rho_G = \sum_i p_i \rho_1^i \otimes \rho_2^i,$$

The separable representation clearly implies that $A_{ij} = {A_{ji}}^*$, which contradicts our assumption. Therefore, graph G associated to the quantum state cannot be written as a convex sum of tensor products of individual subsystems. Hence, the graph G associated to the quantum state is not separable if $A_{ij} \neq {A_{ji}}^*$ and $A_{ij'} \neq {A_{ji'}}^*$. □

Example 5 Consider the graph G_1 associated with an entangled state, and represented as



G_1

The density operator for the graph G_1 is

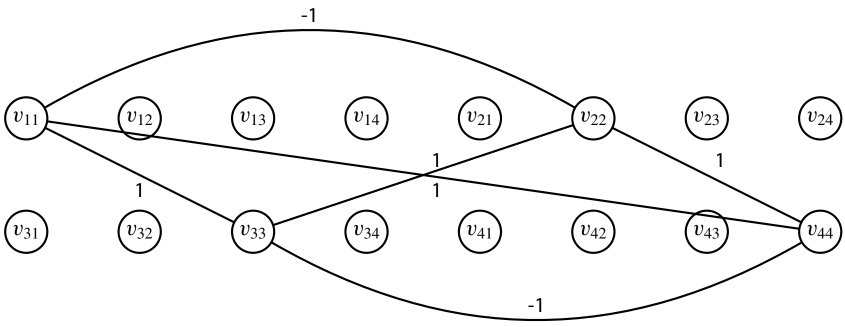
$$\rho_{G_1} = \frac{1}{6}\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix},$$

and

$$\rho_{G_1}{}^{PT} = \frac{1}{6}\begin{bmatrix} 1 & -1 & 0 & -1 \\ -1 & 3 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ -1 & -1 & 0 & 1 \end{bmatrix}.$$

Here, $\rho_{G_1} \neq \rho_{G_1}{}^{PT}$ and blocks of ρ_{G_1} are not symmetric matrix after interchanging columns and corresponding rows. Hence, the state associated with G_1 is entangled.

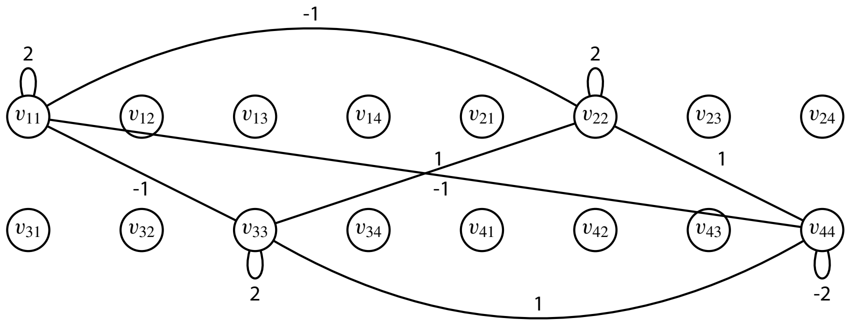
Example 6 Rigolin et al. [27, 28] have introduced maximally entangled four qubit states, but following our Theorems (4.4) and (4.7), one can easily show that the states are separable with an absence of genuine four-qubit entanglement. The graph G_2 depicted below serves as an example of the above theorem.



G_2

A brief description of Example 6 above is presented in the Appendix.

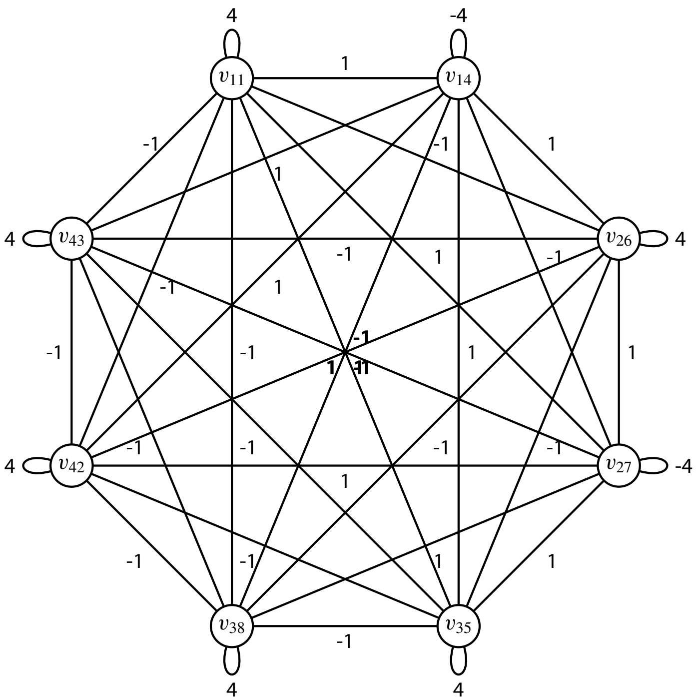
Example 7 The graph G_3 depicted below also serves as an example of the above Theorem 4.7.



G_3

Clearly, the state associated with the graph G_3 is entangled as also briefly demonstrated in the Appendix.

Example 8 As another illustration of the theorem, we consider the graph G_4 where the isolated vertices are not considered.



G_4

Similar to the previous example, in this case also the state associated with G_4 is an entangled state.

Example 9 Let us consider the state [23] $|W\rangle = \frac{1}{\sqrt{3}}(|011\rangle + e^{i\frac{4\pi}{3}}|101\rangle + e^{i\frac{2\pi}{3}}|110\rangle)$. Therefore, the density operator corresponding to the state $|W\rangle$ can be represented as

$$\rho = \frac{1}{3}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & e^{-i\frac{4\pi}{3}} & e^{-i\frac{2\pi}{3}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\frac{4\pi}{3}} & 0 & 1 & e^{i\frac{2\pi}{3}} & 0 \\ 0 & 0 & 0 & e^{i\frac{2\pi}{3}} & 0 & e^{-i\frac{2\pi}{3}} & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Considering ρ to be a block matrix, one can clearly show that all blocks are not Hermitian. Hence, using Theorem 4.7, the given state is an entangled state.

Example 10 We now consider another state represented in [23] as $|z\rangle = \frac{1}{2}(|001\rangle + |010\rangle + |100\rangle + e^{2i\phi}|111\rangle)$. Using the above state, one can express the density operator as

$$\rho = \frac{1}{4}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & e^{-2i\phi} \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & e^{-2i\phi} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & e^{-2i\phi} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{2i\phi} & e^{2i\phi} & 0 & e^{2i\phi} & 0 & 0 & 1 \end{bmatrix}$$

Similar to the previous example, if we consider ρ to be a 2×2 block matrix, then the blocks are not Hermitian. Therefore, using Theorem 4.7, the given state is an entangled state.

Example 11 Here, we further extend our discussion by considering the state $\rho(T)$ from [38], represented as $\rho(T) = \frac{1}{Z}$

$$\begin{bmatrix} e^{\frac{-\beta J}{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{2}e^{\frac{\beta(J-\delta)}{2}}(1+e^{\beta\delta}) & \frac{1}{2}e^{i\theta}e^{\frac{\beta(J-\delta)}{2}}(1-e^{\beta\delta}) & 0 \\ 0 & \frac{1}{2}e^{-i\theta}e^{\frac{\beta(J-\delta)}{2}}(1-e^{\beta\delta}) & \frac{1}{2}e^{\frac{\beta(J-\delta)}{2}}(1+e^{\beta\delta}) & 0 \\ 0 & 0 & 0 & e^{\frac{-\beta J}{2}} \end{bmatrix}$$

where $Z = 2e^{-\frac{\beta J}{2}}[1 + e^{\beta J} cosh\frac{\beta\delta}{2}]$, $\beta = \frac{1}{kT}$, and $\delta = 2J\sqrt{1 + D^2}$.
In this case also, if we consider ρ to be a 2×2 block matrix then the resultant blocks are not Hermitian. Clearly, the density operator cannot be written as a convex sum of tensor products of density operators. Using Theorem 4.7, if $e^{\frac{\beta(J-\delta)}{2}}(1 - e^{\beta\delta}) \neq 0$ then the state is entangled. Alternately, as discussed above, for separability we must have $e^{\frac{\beta(J-\delta)}{2}}(1 - e^{\beta\delta}) = 0$ which is possible only if $J = 0$. Theorem 4.4 further leads us to $E_{bb} = A_{bb} - A_{bc} \geq 0$ confirming that the state is a separable state if $e^{\frac{\beta(J-\delta)}{2}}(1 - e^{\beta\delta}) = 0$.
Similarly, using Theorem 4.1, for $J = 0$ the density operator $\rho(T)$ can be re-expressed as $\rho(T) = \frac{1}{4}\begin{bmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&1&0 \\ 0&0&0&1 \end{bmatrix}$. Here $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4$ where λ_i are eigen values and $\lambda_1 < \lambda_2 + \lambda_3$, therefore, using Theorem 4.1, the state is a separable state for $J = 0$.

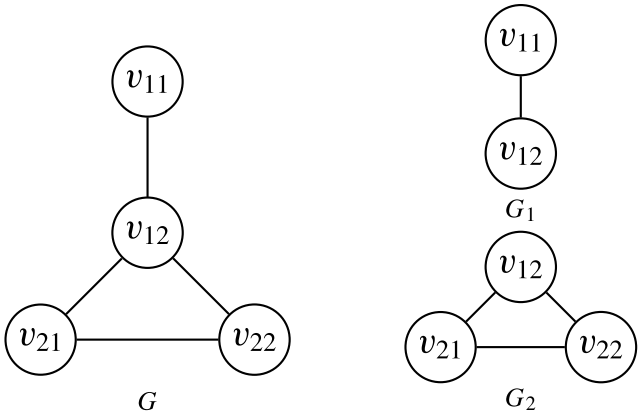
Corollary 4.8 *Let G be a simple graph on 2^n vertices with at least two edges associated with an n-qubit state and ρ_G be the density operator. If $\rho_G \neq {\rho_G}^{PT}$ then G is associated with an entangled state.*

Corollary 4.9 *Let G be a simple graph on 2^n vertices associated with an n-qubit state. If the Laplacian matrix of G is expressed as $L(G) = \left[\begin{array}{c|c} L_1 & 0 \\ \hline 0 & L_2 \end{array}\right] + \left[\begin{array}{c|c} D & B \\ \hline B & D \end{array}\right]$, where D is a diagonal matrix whose elements are row sum of $-B$, then the graph G is associated with a separable state and L_1 and L_2 are Laplacian matrices of subgraph of G.*

4.1 Entanglement and separability of Block graphs

We now proceed to discuss entanglement and separability in another important class of graphs, i.e., block graphs. For a connected graph G, a vertex $v \in V(G)$ is called a *cut-vertex* if $G - v$ is not connected. A maximal connected subgraph of G is called a *block* if it has no cut-vertex. A graph G is known as a *block graph* if every block of G is a complete graph. For example,

Graph	Blocks of graph



$L(G)$	$=L(G_1)+L(G_2)$
$\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix}$	$= \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 0 \\ 0 & 2 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix}$

Theorem 4.10 *Let (G, a) be a weighted block graph on 2^n vertices with k blocks, associated with an n-qubit state. The state associated with the weighted graph (G, a) is entangled if at least one of the blocks of graph is associated with an entangled state.*

Proof Let (G, a) be a weighted block graph having 2^n vertices with k blocks. The Laplacian matrix of the graph (G, a) can be written as $L(G) = L_{G_1} + L_{G_2} + \cdots + L_{G_k}$. Therefore, the density operator of the graph (G, a) is, $\rho_G = \frac{1}{Tr(L_{G_1}+L_{G_2}+\cdots+L_{G_k})}[L_{G_1} + L_{G_2} + \cdots + L_{G_k}]$. The density operator ρ_G can be re-expressed as

$$\begin{aligned}\rho_G = & \frac{Tr(L_{G_1})}{Tr(L_{G_1} + L_{G_2} + \cdots + L_{G_k})}\left\{\frac{1}{Tr(L_{G_1})}[L_{G_1}]\right\} \\ & + \frac{Tr(L_{G_2})}{Tr(L_{G_1} + L_{G_2} + \cdots + L_{G_k})}\left\{\frac{1}{Tr(L_{G_2})}[L_{G_2}]\right\} \\ & + \cdots + \frac{Tr(L_{G_k})}{Tr(L_{G_1} + L_{G_2} + \cdots + L_{G_k})}\left\{\frac{1}{Tr(L_{G_k})}[L_k]\right\}.\end{aligned}$$

Assuming the r^{th} block of the graph (G, a) to be associated with an entangled state suggests that $A_{G_{rij}} \neq (A_{G_{rji}})^*$ where $A_{G_{rij}}$ is ij^{th} block of ρ_{G_r} which is a density operator associated with the r^{th} block of the graph (G, a). Similarly, $A_{G'_{rij}} \neq (A_{G'_{rij}})^*$

where $A_{G'_{r ij}}$ is ij^{th} block of $\rho_{G'_r}$ such that $\rho_{G'_r}$ is a density operator after interchanging columns C_i with C_j, and corresponding rows R_i with R_j in ρ_{G_r}. Clearly, $A_{ij} \neq (A_{ji})^*$ and $A_{ij'} \neq (A_{ji'})^*$, where A_{ij} is ij^{th} block of ρ_G and $A_{ij'}$ is ij^{th} block of $\rho_{G'}$ where $\rho_{G'}$ represents a density operator after interchanging columns C_i with C_j, and corresponding rows R_i with R_j in ρ_G. Therefore, using Theorem (4.7), the weighted block graph is associated with an entangled state. □

Theorem 4.11 *Let (G, a) be a weighted block graph on 2^n vertices associated with a $(n = p + q)$ qubit state. The state associated with the weighted graph (G, a) is separable if vertex sets of blocks are $\{v_{11}, v_{12}, \ldots, v_{12^q}\}$, $\{v_{21}, v_{22}, \ldots, v_{22^q}\}$, $\ldots$,$\{v_{2^p1}, v_{2^p2}, \ldots, v_{2^p2^q}\}$, and $\{v_{ij}, v_{kl}\}$ for $i \neq k$ where $k \neq 2^p - (i-1)$ and $l \neq 2^q - (j-1)$.*

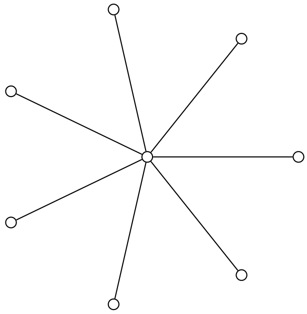
Proof Let (G, a) be a weighted block graph on 2^n vertices associated with a $(n = p + q)$ qubit state. For the vertex sets of blocks , i.e., $\{v_{11}, v_{12}, \ldots, v_{12^q}\}$, $\{v_{21}, v_{22}, \ldots, v_{22^q}\}$,...,$\{v_{2^p1}, v_{2^p2}, \ldots, v_{2^p2^q}\}$, and $\{v_{ij}, v_{kl}\}$ for $i \neq k$ where $k \neq 2^p - (i-1)$ and $l \neq 2^q - (j-1)$, the density operator can be expressed as $\rho_G = \frac{Tr(A)}{Tr(L(G))}\left\{\frac{1}{Tr(A)}[A]\right\} + \frac{Tr(B)}{Tr(L(G))}\left\{\frac{1}{Tr(B)}[B]\right\}$ where A is a diagonal block matrix which can therefore be expressed as a tensor product. Clearly B can also be expressed as a tensor product by Theorem (4.2), hence the proof. □

Corollary 4.12 *Let G be a simple graph on 2^n vertices associated with an n-qubit state. If every vertex of G has degree $k \geq 2$ and G has no cut-vertex, then the graph G is associated with a separable state*

Proof Let G be a simple graph on 2^n vertices associated with an n-qubit state. If every vertex of G has degree $k \geq 2$ and G has no cut-vertex, then the graph G is connected and $L(G) = \begin{bmatrix} L_1 & 0 \\ 0 & L_1 \end{bmatrix} + \begin{bmatrix} D_1 & B_1 \\ B_1 & D_1 \end{bmatrix}$,
where L_1 is the Laplacian of a subgraph of the simple graph G . D_1 is a diagonal matrix with the i-th diagonal entry equals to sum of absolute value of i-th row (or column) of B_1. Hence the proof. □

4.2 Entanglement and separability of Star graphs (S_n)

We further discuss the properties of star graphs where a star graph (S_n) is a complete bipartite graph on $n + 1$ vertices or n edges, e.g.,



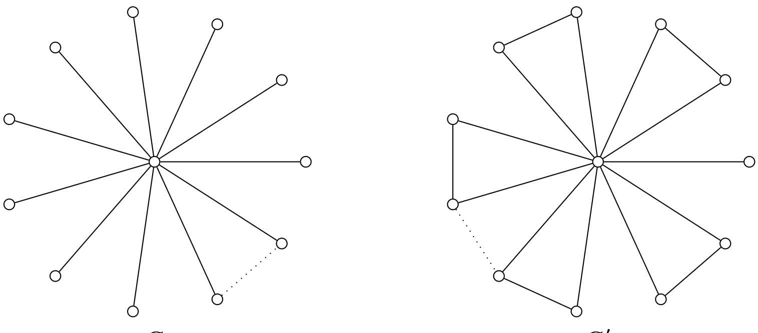
S_8

Theorem 4.13 *Let G be a star graph on 2^m vertices associated with an m-qubit state. If r vertices are deleted from G then the resulting graph on 2^s vertices is associated with an entangled quantum state and* $0 \leq r \leq 2(2^{(m-1)} - 1)$.

Proof Let G be a star graph such that $|V(G)| = 2^m$ $(m \geq 2)$ and $|E(G)| = 2^m - 1$. Since a star graph has cut vertices, it will have blocks that are equal in numbers to the number of edges. By Theorem (4.2) at least one of the blocks of the star graph is associated with an entangled state because of the block containing an edge between v_{ij} and $v_{2^q-(i-1)\ 2^p-(j-1)}$, where $i = 1, 2, \ldots, 2^q$ and $j = 1, 2, \ldots, 2^p$. Therefore, following Theorem (4.10), the state associated with star graph is an entangled state. If r vertices are deleted from G then the resulting graph G'on 2^s vertices will also be a star graph. Since every star graph on 2^m vertices is entangled, G' is also associated with an entangled state. Clearly, $r = 2^m - 2^s = 2^s(2^{(m-s)} - 1)$, where $s = 1, 2, \ldots, m$ which shows that $0 \leq r \leq 2(2^{(m-1)} - 1)$. □

Theorem 4.14 *Let G be a star graph on 2^m vertices. Adding adjacent edges to the graph G results in G′ with blocks having either one edge or three edges. The resultant graph G′ will have at least one block which is associated with an entangled state and entanglement measure of blocks of G′ would not exceed the entangled measure of blocks of G.*

Proof Let G be a star graph on 2^m vertices and G' be the resultant graph after adding r adjacent edges to the graph G, where $1 \leq r \leq \frac{|E(G)|-1}{2}$.



G G'

The graph G' contains cut vertices and a minimum of $\frac{|E(G)|+1}{2}$ blocks. Since one block ${G_k}'$ of the graph G' contains the edge between vertices v_{ij} and $v_{2^q-(i-1)\ 2^p-(j-1)}$, where $i = 1, 2, \ldots, 2^q$ and $j = 1, 2, \ldots, 2^p$, thus by Theorem (4.2) and (4.7), ${G_k}'$ is associated with an entangled state. Further, we know that the degree of entanglement of a simple graph is equal to $\frac{1}{|E(G)|}$ for an entangled state and 0 for a separable state [20]; therefore, the degree of entanglement for all blocks of G' can either be 0, or 1 or $\frac{1}{3}$, where the degree of entanglement for all blocks of G is either 0 or 1. Hence proved. □

5 Conclusion

In this article, we demonstrated effective entanglement and separability conditions for weighted, block and star graphs associated with n-qubit states. Our analysis led us to describe entanglement properties of multi-qubit states utilizing characteristics of graphs and density operators. The study presented here is important from the perspective that characterization of weighted, block and star graphs in terms of entanglement and separability is relatively unexplored in comparison with simple graphs. We believe that the results obtained in this article will allow one to address entanglement and separability problem for these classes of graphs in an effective manner.

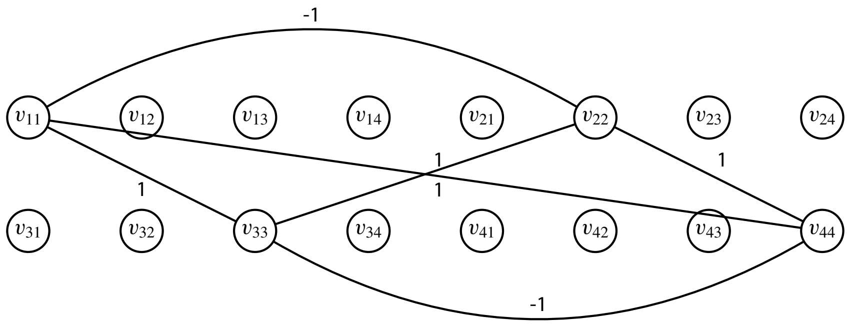
Acknowledgements The authors are grateful to Ranveer Singh and Satish Sangwan for their valuable comments and suggestions. The authors are also grateful to IIT Jodhpur for providing the research infrastructure. On behalf of all authors, the corresponding author states that there is no conflict of interest.

Data Availability statement All data generated or analyzed during this study are included in this published article.

6 Appendix

6.1 A brief explanation of Examples (6) and (7)

1. Explanation of the example (6)



G_2

The density operator for the graph G_2 can be represented as

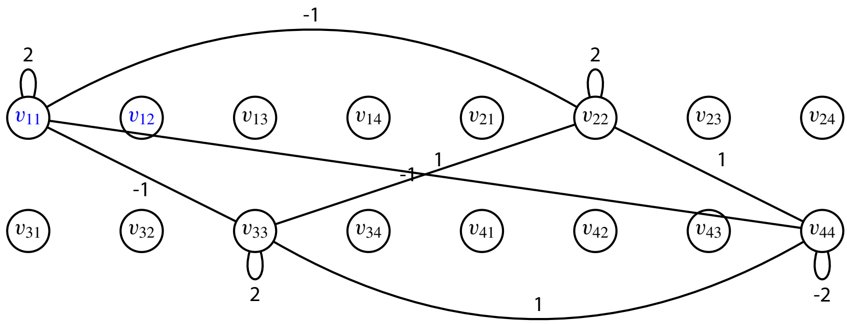
$$\rho_{G_2} = \frac{1}{4}\begin{bmatrix}
1&0&0&0&0&1&0&0&0&0&-1&0&0&0&0&-1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&0&0&1&0&0&0&0&-1&0&0&0&0&-1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
-1&0&0&0&0&-1&0&0&0&0&1&0&0&0&0&1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
-1&0&0&0&0&-1&0&0&0&0&1&0&0&0&0&1
\end{bmatrix}$$

Using ρ_{G_2} , one can verify that $\rho_{G_2} \neq {\rho_{G_2}}^{PT}$. Therefore, interchanging columns C_9 with C_{11}, and C_{14} with C_{16} and corresponding rows R_9 with R_{11} and R_{14} with R_{16}, we have

$$\rho_{G_2} \cong {\rho_{G_2}}' = \frac{1}{4}\begin{bmatrix}
1&0&0&0&0&1&0&0&-1&0&0&0&0&-1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&0&0&1&0&0&-1&0&0&0&0&-1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
-1&0&0&0&0&-1&0&0&1&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
-1&0&0&0&0&-1&0&0&1&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{bmatrix}.$$

Here, we can see that blocks are symmetric, satisfying the Theorem 4.4. Hence, the state associated with the graph G_2 is separable.

2. Explanation of the example (7)



G_3

Similar to the previous case, the density operator for the graph G_3 is expressed as

$$\rho_{G_3} = \frac{1}{4}\begin{bmatrix}
1&0&0&0&0&1&0&0&0&0&1&0&0&0&0&-1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&0&0&1&0&0&0&0&1&0&0&0&0&-1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&0&0&1&0&0&0&0&1&0&0&0&0&-1\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
-1&0&0&0&0&-1&0&0&0&0&-1&0&0&0&0&1
\end{bmatrix},$$

In this case, we can see that we cannot get the symmetric blocks by interchanging the columns and corresponding rows. Therefore, the state associated with the graph G_3 is entangled.

6.2 Decomposition of the Laplacian matrix of a simple graph *G*

Every Laplacian matrix can be decomposed as a sum of Laplacian matrices of subgraphs (G_1, G_2, and G_3) of a graph G [24].

We have

$$L=\begin{bmatrix}\sum_{j=1}^{n}a_{1j} & -a_{12} & \dots & -a_{1n}\\ -a_{21} & \sum_{j=1}^{n}a_{2j} & \dots & -a_{2n}\\ \vdots & \vdots & \vdots & \vdots\\ -a_{n1} & -a_{n2} & \dots & \sum_{j=1}^{n}a_{nj}\end{bmatrix}.$$

It is easy to see that $L(G)$ can be rewritten as

$$L=\begin{bmatrix}\sum_{j=1}^{\frac{n}{2}}a_{1j} & -a_{12} & \dots-a_{1\frac{n}{2}} & 0\;0\dots 0\\ -a_{21} & \sum_{j=1}^{\frac{n}{2}}a_{2j} & \dots-a_{2\frac{n}{2}} & 0\;0\dots 0\\ \vdots & \vdots & \vdots & \vdots\;\vdots\;\vdots\\ -a_{\frac{n}{2}1} & -a_{\frac{n}{2}2} & \dots\sum_{j=1}^{\frac{n}{2}}a_{\frac{n}{2}j} & 0\;0\dots 0\\ 0 & 0 & \dots & 0\;0\dots 0\\ 0 & 0 & \dots & 0\;0\dots 0\\ \vdots & \vdots & \vdots & \vdots\;\vdots\;\vdots\\ 0 & 0 & \dots & 0\;0\dots 0\end{bmatrix}$$

$$+\begin{bmatrix}0\;0\dots 0\;0 & 0 & \dots & 0 & \\ 0\;0\dots 0\;0 & 0 & \dots & 0 & \\ \vdots\;\vdots\;\vdots\;\vdots & \vdots & \vdots & & \\ 0\;0\dots 0\;0 & \dots & 0 & & \\ 0\;0\;\dots\;0 & \sum_{j=\frac{n}{2}+1}^{n}a_{\frac{n}{2}+1j} & -a_{\frac{n}{2}+1\frac{n}{2}+2} & \dots-a_{\frac{n}{2}+1n} & \\ 0\;0\;\dots\;0 & -a_{\frac{n}{2}+2\frac{n}{2}+1} & \sum_{j=\frac{n}{2}+1}^{n}a_{\frac{n}{2}+2j} & \dots-a_{\frac{n}{2}+2n} & \\ \vdots\;\vdots\;\vdots\;\vdots & \vdots & \vdots & & \\ 0\;0\;\dots\;0 & -a_{n\frac{n}{2}+1} & -a_{n\frac{n}{2}+2} & \dots\;0 & \sum_{j=\frac{n}{2}+1}^{n}a_{nj}\end{bmatrix}$$

$$+\begin{bmatrix}\sum_{j=\frac{n}{2}+1}^{n}a_{1j} & \dots & 0 & -a_{1\frac{n}{2}+1} & \dots & -a_{1n}\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ 0 & \dots & \sum_{j=\frac{n}{2}+1}^{n}a_{\frac{n}{2}j} & -a_{\frac{n}{2}\frac{n}{2}+1} & \dots & -a_{\frac{n}{2}n}\\ -a_{\frac{n}{2}+11} & \dots & -a_{\frac{n}{2}+1\frac{n}{2}} & \sum_{j=1}^{\frac{n}{2}}a_{\frac{n}{2}+1j} & \dots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ -a_{n1} & \dots & -a_{n\frac{n}{2}} & 0 & \dots & \sum_{j=1}^{\frac{n}{2}}a_{nj}\end{bmatrix}.$$

To summarize, $L(G) = \begin{bmatrix} L_1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & L_2 \end{bmatrix} + \begin{bmatrix} D_1 & B_1 \\ B_2 & D_2 \end{bmatrix}$, where L_1 and L_2 are also Laplacian of simple graphs and D_1 and D_2 are diagonal matrices with the i-th diagonal entry equals to the sum of absolute value of i-th row sum of B_1 and B_2.

References

1. Adhikari, B., Banerjee, S., Adhikari, S., Kumar, A.: Laplacian matrices of weighted digraphs represented as quantum states. Quantum Inf. Process. **16**(3), 79 (2017)
2. Bennett, C.H., DiVincenzo, D.P., Smolin, J.A., Wootters, W.K.: Mixed-state entanglement and quantum error correction. Phys. Rev. A **54**(5), 3824 (1996)
3. Berkolaiko, G., Kuchment, P.: Introduction to Quantum Graphs. Number 186. American Mathematical Society (2013)
4. Braunstein, S.L., Ghosh, S., Mansour, T., Severini, S., Wilson, R.C.: Some families of density matrices for which separability is easily tested. Phys. Rev. A **73**(1), 012320 (2006)
5. Braunstein, S.L., Ghosh, S., Severini, S.: The Laplacian of a graph as a density matrix: a basic combinatorial approach to separability of mixed states. Ann. Comb. **10**(3), 291–317 (2006)
6. Bruss, D., Leuchs, G.: Quantum Information: From Foundations to Quantum Technology Applications. Wiley, New York (2019)
7. Coffman, V., Kundu, J., Wootters, W.K.: Distributed entanglement. Phys. Rev. A **61**(5), 052306 (2000)
8. Dür, W., Aschauer, H., Briegel, H.-J.: Multiparticle entanglement purification for graph states. Phys. Rev. Lett. **91**(10), 107903 (2003)
9. Dür, W., Vidal, G., Cirac, J.I.: Three qubits can be entangled in two inequivalent ways. Phys. Rev. A **62**(6), 062314 (2000)
10. Dutta, S., Adhikari, B., Banerjee, S.: A graph theoretical approach to states and unitary operations. Quantum Inf. Process. **15**(5), 2193–2212 (2016)
11. Dutta, S.: Bipartite separability and nonlocal quantum operations on graphs. Phys. Rev. A **94**(1), 012306 (2016)
12. Eisert, J., Plenio, M.B.: Introduction to the basics of entanglement theory in continuous-variable systems. Int. J. Quantum Inf. **1**(04), 479–506 (2003)
13. Hall, B.C.: Quantum Theory for Mathematicians, vol. 267. Springer, Berlin (2013)
14. Hall, M.J.W.: Random quantum correlations and density operator distributions. Phys. Lett. A **242**(3), 123–129 (1998)
15. Hassan, A.S.M., Joag, P.S.: A combinatorial approach to multipartite quantum systems: basic formulation. J. Phys. A Math. Theor. **40**(33), 10251 (2007)
16. Hildebrand, R., Mancini, S., Severini, S.: Combinatorial Laplacians and positivity under partial transpose. Math. Struct. Comput. Sci. **18**(1), 205–219 (2008)
17. Horodecki, M., Horodecki, P., Horodecki, R.: Separability of n-particle mixed states: necessary and sufficient conditions in terms of linear maps. Phys. Lett. A **283**(1–2), 1–7 (2001)
18. Horodecki, R., Horodecki, P., Horodecki, M., Horodecki, K.: Reviews of modern physics. Quantum Entangl **81**(2), 865 (2009)
19. Hou, Q.-H., Mansour, T., Severini, S.: Partial transposes of permutation matrices. Integers Electron J Combin Number Theory **8**(A49), A49 (2008)
20. Joshi, A., Singh, R., Kumar, A.: Concurrence and three-tangle of the graph. Quantum Inf. Process. **17**(12), 327 (2018)
21. Lohmayer, R., Osterloh, A., Siewert, J., Uhlmann, A.: Entangled three-qubit states without concurrence and three-tangle. Phys. Rev. Lett. **97**(26), 260502 (2006)
22. Meenakshi, A.R., Rajian, C.: On a product of positive semidefinite matrices. Linear Algebra Appl. **295**(1–3), 3–6 (1999)
23. Milivojević, M.: Maximal thermal entanglement using three-spin interactions. Quantum Inf. Process. **18**(2), 1–14 (2019)
24. Newman, M.W.: The Laplacian spectrum of graphs (2001)
25. Nielsen, M.A., Chuang, I.: Quantum computation and quantum information (2002)
26. Nielsen, M.A., Chuang, I.L.: Quantum computation and quantum information (2000)

27. Rigolin, G.: Superdense coding using multipartite states. arXiv:hep/0407193 (2004)
28. Rigolin, G.: Quantum teleportation of an arbitrary two-qubit state and its relation to multipartite entanglement. Phys. Rev. A **71**(3), 032303 (2005)
29. Wang, B.-Y., Gong, M.-P.: Some eigenvalue inequalities for positive semidefinite matrix power products. Linear Algebra Appl. **184**, 249–260 (1993)
30. Wang, X., Wilde, M.M.: Cost of quantum entanglement simplified. Phys. Rev. Lett. **125**(4), 040502 (2020)
31. Werner, R.F.: Quantum states with Einstein–Podolsky–Rosen correlations admitting a hidden-variable model. Phys. Rev. A **40**(8), 4277 (1989)
32. West, D.B., et al.: Introduction to Graph Theory, vol. 2. Prentice Hall, Upper Saddle River (2001)
33. Wilson, R.J.: Introduction to Graph Theory. Pearson Education, New York (1979)
34. Wootters, W.K.: Entanglement of formation of an arbitrary state of two qubits. Phys. Rev. Lett. **80**(10), 2245 (1998)
35. Wootters, W.K.: Entanglement of formation and concurrence. Quantum Inf. Comput. **1**(1), 27–44 (2001)
36. Wu, P.Y.: Products of positive semidefinite matrices. Linear Algebra Appl. **111**, 53–61 (1988)
37. Zhang, F., Zhang, Q.: Eigenvalue inequalities for matrix product. IEEE Trans. Autom. Control **51**(9), 1506–1509 (2006)
38. Zhang, G.-F.: Thermal entanglement and teleportation in a two-qubit Heisenberg chain with Dzyaloshinski–Moriya anisotropic antisymmetric interaction. Phys. Rev. A **75**(3), 034304 (2007)