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The Laplacian of a Graph as a Density Matrix: A Basic Combinatorial Approach to Separability of Mixed States

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Abstract. We study entanglement properties of mixed density matrices obtained from combinatorial Laplacians. This is done by introducing the notion of the density matrix of a graph. We characterize the graphs with pure density matrices and show that the density matrix of a graph can be always written as a uniform mixture of pure density matrices of graphs. We consider the von Neumann entropy of these matrices and we characterize the graphs for which the minimum and maximum values are attained. We then discuss the problem of separability by pointing out that separability of density matrices of graphs does not always depend on the labelling of the vertices. We consider graphs with a tensor product structure and simple cases for which combinatorial properties are linked to the entanglement of the state. We calculate the concurrence of all graphs on four vertices representing entangled states. It turns out that for these graphs the value of the concurrence is exactly fractional.

Keywords: graph laplacian, density matrix, entanglement

1. Introduction

Quantum information is a field which has been expanding rapidly due to the theoretical successes in fast algorithms, super-dense quantum coding, quantum error correction, teleportation and more. Most of these schemes run off entanglement in quantum states. Although entanglement in pure state systems is relatively "well understood", this is much less so in the case of the so-called mixed quantum states, which are statistical mixtures of pure quantum states. In this paper we aim to make some beginning steps towards improving this situation by focusing our attention to a restricted class of mixed states. The states we study here may be represented as graphs in a natural way. We hope that in this manner we may be able to make powerful statements at least about the class of states represented by what we call *density matrices of graphs*. We find, for example, that certain classes of graphs always represent entangled (separable) states. We also find that a number of considered states have an exactly fractional value of their concurrence — a measure of entanglement of formation in small quantum systems. The representation of a limited class of states by graphs leaves hints in the expressions we find for possibly natural ways to extend certain graph-theoretic concepts to more general objects like signed graphs and weighted graphs.

The paper is divided into six sections. In Section 2, we introduce the notion of the density matrix of a graph. Theorem 2.5 characterizes the graphs with pure density matrices. Theorem 2.8 shows that the density matrix of a graph can be written as a uniform mixture of pure density matrices of graphs. In Section 3, we consider the von Neumann entropy of density matrices of graphs. Theorem 3.2 calculates the minimum and maximum von Neumann entropy that the density matrix of a graph can have, and determines the graphs for which these values are attained. Theorem 3.4 studies the von Neumann entropy of the disjoint union of cycles. In Section 4, we discuss separability. We label the $n = pq$ vertices of a graph by an ordered pair of indices, where the first index can take p different values and the second index can take q different values. Theorem 4.2 points out that separability of the density matrix of a graph is generally dependent on the labelling of the vertices of the graph. This does not hold for complete graphs, which represent separable states (Lemma 4.7), and star graphs, which represent entangled states (Theorem 4.11). Theorem 4.8 shows that if a graph is a tensor product then its density matrix is separable, and the converse of it is not necessarily true. After having introduced the notion of the entangled edge, we prove that if all the entangled edges of a graph on $n = 2p$ vertices form a perfect matching, then the density matrix of the graph is separable in $\mathbb{C}^2 \otimes \mathbb{C}^p$ (Theorem 4.17). We observe that strongly-regular graphs and transitive graphs can have entangled or separable density matrices (Corollary 4.27). We calculate the concurrence of all graphs on four vertices representing entangled states. It turns out that for these graphs the value of the concurrence is exactly fractional. In Section 5, we describe the quantum operations that implement graph transformations like adding or deleting a vertex or an edge. In Section 6, we state open problems and conjectures. The paper is relatively self-contained. Our references on graph theory and quantum mechanics are [2] and [8], respectively.

2. The Density Matrix of a Graph

2.1. Definition

A *graph* $G = (V, E)$ is a pair defined in the following way: V (or $V(G)$) is a non-empty and finite set whose elements are called *vertices*; E (or $E(G)$) is a non-empty set of unordered pairs of vertices, which are called *edges*. A *loop* is an edge of the form $\{v_i, v_i\}$, for some vertex v_i. We assume that $E(G)$ does not contain only loops. A graph G is said to be *on n vertices* if $|V(G)| = n$. The *adjacency matrix* of a graph G on n vertices is an $n \times n$ matrix, denoted by $M(G)$, having rows and columns labeled by the vertices of G, and the (i, j)-entry defined as follows:

$$[M(G)]_{i,j} = \begin{cases} 1, & \text{if } \{v_i, v_j\} \in E(G); \\ 0, & \text{if } \{v_i, v_j\} \notin E(G). \end{cases}$$

Two distinct vertices v_i and v_j are said to be *adjacent* if $\{v_i, v_j\} \in E(G)$. The *degree* of a vertex $v_i \in V(G)$, denoted by $d_G(v_i)$, is the number of edges adjacent to v_i. Two adjacent vertices are also said to be *neighbours*. The *degree-sum* of G is defined and denoted by $d_G = \sum_{i=1}^{n} d_G(v_i)$. Note that $d_G = 2|E(G)|$. The *degree matrix* of G is an $n \times n$ matrix, denoted by $\Delta(G)$, having the (i, j)-entry defined as follows:

$$[\Delta(G)]_{i,j} = \begin{cases} d_G(v_i), & \text{if } i = j; \\ 0, & \text{if } i \neq j. \end{cases}$$

The *combinatorial laplacian matrix* of a graph G (for short, *laplacian*) is the matrix

$$L(G) \stackrel{def}{=} \Delta(G) - M(G).$$

Notice that $L(G)$ does not change if we add or delete loops from G. According to our definition of the graph, $L(G) \neq 0$.

Example 2.1. Let I_n and J_n be the $n \times n$ identity matrix and the $n \times n$ all-ones matrix, respectively. The *complete graph* on n vertices, denoted by K_n, is defined to be the graph with adjacency matrix $(J_n - I_n)$. Then

$$L(K_n) = (n-1)I_n - J_n + I_n = nI_n - J_n.$$

In standard quantum mechanics (that is the Hilbert space formulation of quantum mechanics), the state of a quantum mechanical system associated to the n-dimensional Hilbert space $\mathcal{H} \cong \mathbb{C}^n$ is identified with an $n \times n$ positive semidefinite, trace-one, Hermitian matrix, called a *density matrix*. It is easy to observe that the laplacian of a graph is symmetric and positive semidefinite. The laplacian of a graph G, scaled by the degree-sum of G, has trace one and it is then a density matrix. This observation leads to the following definition.

Definition 2.2. [The density matrix of a graph] *The* density matrix of a graph G *is the matrix*

$$\sigma(G) \stackrel{def}{=} \frac{1}{d_G} L(G).$$

Example 2.3. The density matrix of K_n (cf. Example 2.1) is

$$\sigma(K_n) = \frac{1}{n(n-1)} (nI_n - J_n).$$

2.2. Pure States and Mixed States

Let $\mathrm{tr}(A)$ be the trace of a matrix A. A density matrix ρ is said to be *pure* if $\mathrm{tr}(\rho^2) = 1$, and *mixed*, otherwise. Theorem 2.5 gives a necessary and sufficient condition on a graph G for $\sigma(G)$ to be pure. We first provide some terminology and state an easy lemma. A graph G is said to have k *components*, $G_1, G_2, \ldots, G_k$, and in such a case we write $G = G_1 \uplus G_2 \uplus \cdots \uplus G_k$, if there is an ordering of $V(G)$, such that $M(G) = \bigoplus_{i=1}^{k} M(G_i)$. When $k = 1$, G is said to be *connected*. From now on, we denote by $\lambda_1(A), \lambda_2(A), \ldots, \lambda_k(A)$ the k different eigenvalues of a Hermitian matrix A in increasing order. The set of the eigenvalues of A together with their multiplicities is called the *spectrum* of A.

Lemma 2.4. *The density matrix of a graph G has a zero eigenvalue whose multiplicity is equal to the number of components of G.*

Proof. Given a graph G, it is a direct consequence of Definition 2.2 that

$$\lambda_i(\sigma(G)) = \frac{\lambda_i(L(G))}{d_G}.$$

It is well-known that $L(G)$ has a zero eigenvalue whose multiplicity is equal to the number of components of G [2]. ∎

Theorem 2.5. *The density matrix of a graph G is pure if and only if* $G = K_2$ *or* $G = K_2 \uplus v_1 \uplus v_2 \uplus \cdots \uplus v_l$*, for some vertices* $v_1, v_2, \ldots, v_l$. (*These vertices are with or without loops.*)

Proof. Let G be a graph on n vertices. Suppose that $\sigma(G)$ is pure. By the definition of the pure density matrix, the different eigenvalues of $\sigma(G)$ are $\lambda_1(\sigma(G)) = 0$ and $\lambda_2(\sigma(G)) = 1$. Moreover, $\lambda_1(\sigma(G)) = 0$ has multiplicity $(n-1)$. Then, by Lemma 2.4, the number of components of G is $(n-1)$. Since $|V(G)| = n$, it follows that $G = K_2 \uplus v_1 \uplus v_2 \uplus \cdots \uplus v_l$, where $l = n-2$. ∎

The next definition is based on the theorem.

Definition 2.6. [Pure density matrix of a graph] *Let G be a graph on* $n \geq 2$ *vertices. The density matrix of graph G is said to be* pure *if* $G = K_2 \uplus v_1 \uplus v_2 \uplus \cdots \uplus v_{n-2}$*, for some vertices* $v_1, v_2, \ldots, v_{n-2}$. (*These vertices are with or without loops.*)

Example 2.7. The density matrix

$$\sigma(K_2) = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

is pure. In fact, $\lambda_1(\sigma(K_2)) = 0$ and $\lambda_2(\sigma(K_2)) = 1$.

A graph H is said to be a *factor* of a graph G, if $V(H) = V(G)$ and there exists a graph H' such that $V(H') = V(G)$ and $M(G) = M(H) + M(H')$.

Theorem 2.8. *The density matrix of a graph is a uniform mixture of pure density matrices.*

Proof. Let G be a graph on n vertices $v_1, v_2, \ldots, v_n$, having edges $\{v_{i_1}, v_{j_1}\}, \{v_{i_2}, v_{j_2}\}, \ldots, \{v_{i_m}, v_{j_m}\}$, where $1 \leq i_1, j_1, i_2, j_2, \ldots, i_m, j_m \leq n$. Let $H_{i_k j_k}$ be the factor of G such that

$$\left[M(H_{i_k j_k})\right]_{u,w} = \begin{cases} 1, & \text{if } u = i_k \text{ and } w = j_k \text{ or } w = i_k \text{ and } u = j_k; \\ 0, & \text{otherwise.} \end{cases} \tag{2.1}$$

By Theorem 2.5, the density matrix $\sigma\left(H_{i_k j_k}\right) = \frac{1}{2}\left(\Delta\left(H_{i_k j_k}\right) - M\left(H_{i_k j_k}\right)\right)$ is pure. Since

$$\Delta(G) = \sum_{k=1}^{m} \Delta\left(H_{i_k j_k}\right) \quad \text{and} \quad M(G) = \sum_{k=1}^{m} M\left(H_{i_k j_k}\right),$$

we can write

$$\sigma(G) = \frac{1}{2m}\left(\Delta(G) - M(G)\right) = \frac{1}{m}\sum_{k=1}^{m} \sigma\left(H_{i_k j_k}\right), \tag{2.2}$$

which is then a uniform mixture of pure density matrices. ∎

Example 2.9. Consider a graph G defined as follows: $V(G) = \{1, 2, 3\}$ and $E(G) = \{e = \{1, 2\}, f = \{2, 3\}\}$. Then

$$M\left(H_{1_e 2_e}\right) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad M\left(H_{2_f 3_f}\right) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

and

$$\sigma(G) = \frac{1}{2}\left(\sigma\left(H_{1_e 2_e}\right) + \sigma\left(H_{2_f 3_f}\right)\right) = \begin{bmatrix} \frac{1}{4} & -\frac{1}{4} & 0 \\ -\frac{1}{4} & \frac{1}{2} & -\frac{1}{4} \\ 0 & -\frac{1}{4} & \frac{1}{4} \end{bmatrix}.$$

3. von Neumann Entropy

The *von Neumann entropy* of an $n \times n$ density matrix ρ is

$$S(\rho) \stackrel{def}{=} -\sum_{i=1}^{n} \lambda_i(\rho) \log_2 \lambda_i(\rho).$$

It is conventional to define $0 \log_2 0 = 0$. The von Neumann entropy is a quantitative measure of mixedness of the density matrix ρ.

Remark 3.1. The *q-entropy* of an $n \times n$ density matrix ρ is $(\mathrm{tr}(\rho^q))^{1/q}$. q-Entropies are a family of measures of mixedness for density matrices. In general, in the limit $q \to \infty$, q-entropies depend only on the largest eigenvalue of ρ, and we have $\lim_{q\to\infty}(\mathrm{tr}(\rho^q))^{1/q} = \lambda_n(\rho)$. This eigenvalue can be considered itself as a measure of mixedness [1]. If ρ is the density matrix of a graph, a tight upper-bound on $\lambda_n(\rho)$ is known [11].

3.1. Maximum and Minimum

Theorem 3.2. *Let G be a graph on n vertices. Then*

(1) $\max_G S(\sigma(G)) = \log_2(n-1) = S(\sigma(K_n))$;

(2) $\min_G S(\sigma(G)) = 0$ *and this value is attained if* $\sigma(G)$ *is pure.*

Proof. (1) By Lemma 2.4, $\sigma(G)$ has an eigenvalue zero with multiplicity at least one. Since G is on n vertices, the support of $\sigma(G)$ has dimension less than or equal to $(n-1)$. Any $n \times n$ density matrix having dimension of support less than or equal to $(n-1)$, can not have von Neumann entropy greater than $\log_2(n-1)$. The eigenvalues of $\sigma(K_n)$ are $\lambda_1(\sigma(K_n)) = 0$, with multiplicity 1, and $\lambda_2(\sigma(K_n)) = \frac{1}{(n-1)}$, with multiplicity $(n-1)$. Then

$$S(\sigma(K_n)) = -\sum \frac{1}{n-1} \log_2 \frac{1}{n-1} = \log_2(n-1).$$

(2) Since G is a graph on n vertices, the maximum multiplicity of the zero eigenvalue of $\sigma(G)$ is $(n-1)$; the other eigenvalue of $\sigma(G)$ is necessarily one. This is the case when $\sigma(G)$ is pure. When $\sigma(G)$ is pure, $S(\sigma(G)) = 0$. ∎

3.2. Regular Graphs

Two graphs G and H are said to be *L-cospectral* if $L(G)$ and $L(H)$ have the same spectrum; σ-*cospectral* if $\sigma(G)$ and $\sigma(H)$ have the same spectrum. Two graphs G and H are said to be *isomorphic*, and in such a case we write $G \cong H$, if there is an *isomorphism* between $V(G)$ and $V(H)$, that is there is a permutation matrix P, such that $PM(G)P^{\intercal} = M(H)$. If $G \cong H$ then G and H are L-cospectral and σ-cospectral, but the converse is not necessarily true. Two graphs are L-cospectral and σ-cospectral if and only if they have the same degree sum. Now, a graph is said to be *regular* if each of its vertices has the same degree. A *d-regular* graph is a regular graph whose degree of the vertices is d. If G is a d-regular graph on n vertices, then $\lambda_i(L(G)) = d - \lambda_i(M(G))$ and $\lambda_i(\sigma(G)) = \frac{d-\lambda_i(M(G))}{dn}$, because $d_G = dn$. So, G and H are L-cospectral d-regular graphs if and only if they are σ-cospectral. Now, let us consider a d-regular graph G. Let us write $\sigma_i = \lambda_i(\sigma(G))$ and $\mu_i = \lambda_i(M(G))$. Let m_i be the multiplicity of the i-th eigenvalue of $M(G)$. This is also the multiplicity of the i-th eigenvalue of $\sigma(G)$, given that G is regular. The von Neumann entropy of G is then given by

$$\begin{aligned}
S(\sigma(G)) &= -\sum_{i=1}^{k} m_i (\sigma_i \log_2 \sigma_i) \\
&= -\frac{1}{d \cdot n} \sum_{i=1}^{k} m_i [(d-\mu_i)\log_2(d-\mu_i)] + \frac{\log_2(d \cdot n)}{d \cdot n} \sum_{i=1}^{k} m_i (d-\mu_i) \\
&= -\frac{1}{d \cdot n} \sum_{i=1}^{k} m_i [(d-\mu_i)\log_2(d-\mu_i)] + \log_2(d \cdot n).
\end{aligned}$$

3.3. Cycles

Let Γ be a finite group. Let $S \subset \Gamma$ be a subset of Γ, such that: the set S does not contain the identity element; an element $s \in S$ if and only if $s^{-1} \in S$. Let $\rho_{reg}(g)$ be the (left) regular permutation representation of an element $g \in \Gamma$. The (*left*) *Cayley graph* of Γ *with respect to* S, denoted by $X(\Gamma, S)$, is defined to be the graph with adjacency matrix $M(X(\Gamma, S)) = \sum_{s \in S} \rho_{reg}(s)$. Notice that $X(\Gamma, S)$ is connected if and only if S generates Γ.

Example 3.3. Let $\Gamma = \mathbb{Z}_n$ be the group of the integers modulo n and let $S = \{1, n-1\} \subset \Gamma$. Let $G \cong X(\Gamma, S)$. Then $M(G) = \rho_{reg}(1) + \rho_{reg}(n-1)$. Since S generates Γ, the graph G is connected. The *n-cycle*, denoted by C_n, is a graph on n vertices $v_1, v_2, \ldots, v_n$ and with n edges $\{v_1, v_2\}, \{v_2, v_3\}, \ldots, \{v_{n-1}, v_n\}, \{v_n, v_1\}$. Hence, $G \cong C_n$.

Theorem 3.4. *Let* $G_k = X(\Gamma, S_k)$ *be a Cayley graph, where* $\Gamma = \mathbb{Z}_n$ *and* $S_k = \{k, n-k\} \subset \Gamma$. *Then*

(1) $\max_{G_k} S(\sigma(G_k)) = S(\sigma(C_n))$, *that is when* $\gcd(k, n) = 1$;
(2) $\min_{G_k} S(\sigma(G_k)) = S\left(\sigma\left(C_{\frac{n}{2}}\right)\right)$.

Proof. (1) We begin by observing that, given $S_k = \{k, n-k\}$, with $k = n/p$, $G_k = C_p \uplus C_p \uplus \cdots \uplus C_p$, where C_p is repeated k times. This indicates that the eigenvalues of $M(G_k)$ are the eigenvalues of $M(C_p)$, each repeated k times:

$$\lambda_j(\sigma(G_k)) = \frac{2p \cdot \lambda_j(\sigma(C_p))}{2n},$$

where $1 \le j \le p$, and each $\lambda_j(\sigma(G_k))$ has multiplicity k. Since, it is well-known that $\lambda_j(M(C_p)) = 2\cos(2\pi j/p)$, where $1 \le j \le p$, we have

$$\lambda_j(\sigma(C_p)) = \frac{2 - 2\cos(2\pi j/p)}{2p} = \frac{2\sin^2(\pi j/p)}{p}$$

and

$$\lambda_j(\sigma(G_k)) = \frac{2\sin^2(\pi j/p)}{n}.$$

By writing

$$A_p(j) = \sin^2\left(\frac{\pi j}{p}\right) \log_2\left(\sin^2\left(\frac{\pi j}{p}\right)\right),$$

the von Neumann entropy of $\sigma(G_k)$ is given by

$$S(\sigma(G_k)) = -k\sum_{j=1}^{p} \frac{2}{n} A_p(j) = \log_2 n - 1 - \frac{2}{n}\sum_{j=1}^{p} A_p(j).$$

Because we do not have any closed form of the series $-\sum_{j=1}^{p} A_p(j)$, we use the following approximation, which is very good for large p:

$$-\sum_{j=1}^{p} A_p(j) \simeq -\frac{p}{\pi}\int_0^{\pi} \sin^2 x \log_2\left(\sin^2 x\right) dx = p \cdot C, \tag{3.1}$$

where

$$C = \left(1 - \frac{\log_2 e}{2}\right) \simeq 0.2787.$$

If $p = 1, 2, -\sum_{j=1}^{p} A_p(j) = 0$. So, if $p = 1, 2$ and n is even, $S\left(\sigma\left(G_{n/2}\right)\right) = \log_2 n - 1$. With the use of Equation (3.1), we obtain

$$S(\sigma(G_k)) \simeq \log_2 n - 1 + 2C/k.$$

If $l = n/q$, then

$$S(\sigma(G_k)) - S(\sigma(G_l)) \simeq 2C\left(\frac{1}{k} - \frac{1}{l}\right).$$

It follows that: $S(\sigma(G_k)) > S(\sigma(G_l))$ if $l > k$; $S(\sigma(G_k)) < S(\sigma(G_l))$ if $l < k$. When $k = 1$, then $G_k = C_n$. Therefore, $S(\sigma(C_n)) > S(\sigma(G_l))$, for all $l > 1$.

(2) By the reasoning above, it is sufficient to observe that $S\left(\sigma\left(G_{\frac{n}{2}}\right)\right) = \log_2 n - 1$. ∎

Example 3.5. In the table below, the values of the von Neumann entropy of the Cayley graphs $X(\mathbb{Z}_{12}, S)$, where $|S| = 2$ are given:

G	$S(\sigma(G))$
$X(\mathbb{Z}_{12}, \{1, 11\})$	3.571
$X(\mathbb{Z}_{12}, \{2, 10\})$	3.126
$X(\mathbb{Z}_{12}, \{3, 9\})$	3.084
$X(\mathbb{Z}_{12}, \{4, 8\})$	3.000
$X(\mathbb{Z}_{12}, \{6\})$	2.585

4. Separability

Let S_A and S_B be two quantum mechanical systems, associated to the p-dimensional and q-dimensional Hilbert spaces $\mathcal{H}_A \cong \mathbb{C}_A^p$ and $\mathcal{H}_B \cong \mathbb{C}_B^q$, respectively. The composite system S_{AB}, which consists of the subsystems S_A and S_B, is associated to the Hilbert space $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$, where "$\otimes$" denotes tensor product. The density matrix ρ_{AB} of S_{AB} is said to be *separable* if

$$\rho_{AB} = \sum_{i=1}^{n} \omega_i \rho_A^{(i)} \otimes \rho_B^{(i)},$$

where $\omega_i \geq 0$, for every $i = 1, 2, \ldots, n$, and $\sum_{i=1}^{n} \omega_i = 1$; $\rho_A^{(i)}$ and $\rho_B^{(i)}$ are density matrices acting on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. A density matrix ρ_{AB} is said to be *entangled* if it is not separable. In the Dirac notation, a unit vector in a Hilbert space $\mathcal{H} \cong \mathbb{C}^n$ is denoted by $|\psi\rangle$, where ψ is a label; given the vectors $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$, the linear functional sending $|\psi\rangle$ to the inner product $\langle\varphi|\psi\rangle$ is denoted by $\langle\varphi|$. We write $|\psi\rangle|\varphi\rangle$ for the tensor product $|\psi\rangle \otimes |\varphi\rangle$. A vector of the form $|\psi\rangle|\varphi\rangle$ is called *product state*. For any unit vector $|\psi\rangle \in \mathcal{H}$, the projector on $|\psi\rangle$ is the Hermitian matrix $|\psi\rangle\langle\psi|$ which we denote by $P[|\psi\rangle]$.

4.1. Tensor Product of Graphs

The *tensor product of two graphs* G and H (also known in literature as strong product, cardinal product, etc.), denoted by $G \otimes H$, is the graph whose adjacency matrix is $M(G \otimes H) = M(G) \otimes M(H)$ ([5]). Whenever we consider a graph $G \otimes H$, where G is on p vertices and H is on q vertices, the separability of $\sigma(G \otimes H)$ is described with respect to the Hilbert space $\mathcal{H}_G \otimes \mathcal{H}_H$, where $\mathcal{H}_G$ is the space spanned by the orthonormal basis $\{|u_1\rangle, |u_2\rangle, \ldots, |u_p\rangle\}$ associated to $V(G)$, and $\mathcal{H}_H$ is the space spanned by the orthonormal basis $\{|w_1\rangle, |w_2\rangle, \ldots, |w_q\rangle\}$ associated to $V(H)$. The vertices of $G \otimes H$ are taken as $u_1w_1, u_1w_2, \ldots, u_1w_q, u_2w_1, u_2w_2, \ldots, u_pw_q$. We associate $|u_1\rangle|w_1\rangle$ to u_1w_1, $|u_1\rangle|w_2\rangle$ to $u_1w_2, \ldots, |u_p|w_q\rangle$ to u_pw_q. In conjunction with this, whenever we talk about separability of any graph G on n vertices, $v_1, v_2, \ldots, v_n$, we consider it in the space $\mathbb{C}^p \otimes \mathbb{C}^q$, where $n = pq$. The vectors $|v_1\rangle, |v_2\rangle, \ldots, |v_n\rangle$ are taken as follows: $|v_1\rangle = |u_1\rangle|w_1\rangle, |v_2\rangle = |u_1\rangle|w_2\rangle, \ldots, |v_q\rangle = |u_1\rangle|w_q\rangle, |v_{q+1}\rangle = |u_2\rangle|w_1\rangle, |v_{q+2}\rangle = |u_2\rangle|w_2\rangle, \ldots, |v_{2q}\rangle = |u_2\rangle|w_q\rangle, \ldots, |v_{pq}\rangle = |u_p\rangle|w_q\rangle$. We make use of the notion of *partial transpose* of a density matrix. Let us consider a $pq \times pq$ density matrix ρ_{AB} acting on $\mathbb{C}^p_A \otimes \mathbb{C}^q_B$. Let $\{|v_1\rangle, |v_2\rangle, \ldots, |v_p\rangle\}$ and $\{|w_1\rangle, |w_2\rangle, \ldots, |w_q\rangle\}$ be orthonormal bases of $\mathbb{C}^p_A$ and $\mathbb{C}^q_B$, respectively. The *partial transpose* of ρ_{AB} with respect to the system S_B is the $pq \times pq$ matrix, denoted by $\rho_{AB}^{\mathsf{T}_B}$, and with the $(i, j; i', j')$-th entry defined as follows: $\left[\rho_{AB}^{\mathsf{T}_B}\right]_{i,j;i',j'} = \langle v_i|\langle w_{j'}|\rho_{AB}|v_{i'}\rangle|w_j\rangle$, where $1 \le i, i' \le p$ and $1 \le j, j' \le q$. Regarding separability of ρ_{AB} we have the following criterion [3, 9]:

Criterion 4.1. [Peres-Horodecki Criterion (PH)] If ρ is a density matrix acting on $\mathbb{C}^2 \otimes \mathbb{C}^2$ or $\mathbb{C}^2 \otimes \mathbb{C}^3$, then ρ is separable if and only if ρ^{T_B} is positive semidefinite.

Theorem 4.2. *Let G and H be two graphs on $n = p \cdot q$ vertices. If $\sigma(G)$ is entangled in $\mathbb{C}^p \otimes \mathbb{C}^q$ and $G \cong H$, then $\sigma(H)$ is not necessarily entangled in $\mathbb{C}^p \otimes \mathbb{C}^q$.*

Proof. Let G be a graph on the vertices 1, 2, 3 and 4, having edges $\{1, 2\}$, $\{2, 3\}$ and $\{3, 4\}$. We associate to G the following orthonormal basis: $\{|1\rangle = |1\rangle_A|1\rangle_B, |2\rangle = |2\rangle_A|1\rangle_B, |3\rangle = |1\rangle_A|2\rangle_B, |4\rangle = |2\rangle_A|2\rangle_B\}$. In terms of this basis

$$(\sigma(G))^{\mathsf{T}_B} = \frac{1}{6}\begin{bmatrix} 1 & -1 & 0 & -1 \\ -1 & 2 & 0 & 0 \\ 0 & 0 & 2 & -1 \\ -1 & 0 & -1 & 1 \end{bmatrix},$$

with spectrum $\left\{[1/2], [1/6], \left[(1+\sqrt{2})/6\right], \left[(1-\sqrt{2})/6\right]\right\}$. Since the last eigenvalue is negative, by the PH criterion, $\sigma(P_4)$ is entangled. Consider the graph $H \cong G$. The edges of H are $\{1, 4\}$, $\{4, 3\}$ and $\{3, 2\}$. We associate to H the above orthonormal basis. Then we have

$$(\sigma(H))^{\mathsf{T}_B} = \frac{1}{6}\begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix} = \sigma(H),$$

and so $\sigma(H)$ is separable. ∎

Lemma 4.3. *The density matrix of the tensor product of two graphs is separable.*

Proof. Let G be a graph on n vertices, $v_1, v_2, \ldots, v_n$, and m edges, $\{v_{i_1}, v_{j_1}\}, \{v_{i_2}, v_{j_2}\}, \ldots, \{v_{i_m}, v_{j_m}\}$, where $1 \leq i_1, j_1, i_2, j_2, \ldots, i_m, j_m \leq n$. Let G' be a graph on p vertices, $v_1, v_2, \ldots, v_p$, and q edges, $\{v'_{s_1}, v'_{t_1}\}, \{v'_{s_2}, v'_{t_2}\}, \ldots, \{v'_{s_q}, v'_{t_q}\}$, where $1 \leq s_1, t_1, s_2, t_2, \ldots, s_q, t_q \leq p$. By Theorem 2.8 (Equation (2.2)), we can write

$$\sigma(G) = \frac{1}{m}\sum_{k=1}^{m}\sigma\left(H_{i_k j_k}\right) \quad \text{and} \quad \sigma\left(G'\right) = \frac{1}{q}\sum_{l=1}^{q}\sigma\left(L_{s_l t_l}\right),$$

where $H_{i_k j_k}$ and $L_{s_l t_l}$ are defined according to Equation (2.1). So,

$$\begin{aligned}
\sigma\left(G \otimes G'\right) &= \frac{1}{d_{G\otimes G'}}\left[\Delta\left(G \otimes G'\right) - M\left(G \otimes G'\right)\right] \\
&= \frac{1}{d_{G\otimes G'}}\sum_{k=1}^{m}\sum_{l=1}^{q}\left[\Delta\left(H_{i_k j_k} \otimes L_{s_l t_l}\right) - M\left(H_{i_k j_k} \otimes L_{s_l t_l}\right)\right] \qquad (4.1) \\
&= \frac{1}{m \cdot q}\sum_{k=1}^{m}\sum_{l=1}^{q}\sigma\left(H_{i_k j_k} \otimes L_{s_l t_l}\right) \\
&= \frac{1}{m \cdot q}\sum_{k=1}^{m}\sum_{l=1}^{q}\frac{1}{2}\left[\sigma^{+}\left(H_{i_k j_k}\right) \otimes \sigma\left(L_{s_l t_l}\right) + \sigma\left(H_{i_k j_k}\right) \otimes \sigma^{+}\left(L_{s_l t_l}\right)\right], \qquad (4.2)
\end{aligned}$$

where

$$\sigma^{+}\left(H_{i_k j_k}\right) \stackrel{def}{=} \Delta\left(H_{i_k j_k}\right) - \sigma\left(H_{i_k j_k}\right) \quad \text{and} \quad \sigma^{+}\left(L_{s_l t_l}\right) \stackrel{def}{=} \Delta\left(L_{s_l t_l}\right) - \sigma\left(L_{s_l t_l}\right).$$

Notice that $\sigma^{+}\left(H_{i_k j_k}\right)$ and $\sigma^{+}\left(L_{s_l t_l}\right)$ are density matrices. Let

$$\sigma^{+}(G) \stackrel{def}{=} \frac{1}{m}\sum_{k=1}^{m}\sigma^{+}\left(H_{i_k j_k}\right) \quad \text{and} \quad \sigma^{+}(G') \stackrel{def}{=} \frac{1}{q}\sum_{l=1}^{q}\sigma^{+}\left(L_{s_l t_l}\right).$$

Then

$$\sigma\left(G \otimes G'\right) = \frac{1}{2}\left[\sigma(G) \otimes \sigma^{+}\left(G'\right) + \sigma^{+}(G) \otimes \sigma\left(G'\right)\right]. \qquad (4.3)$$

Since each of $\sigma(G), \sigma^{+}\left(G'\right), \sigma^{+}(G)$ and $\sigma\left(G'\right)$ is a uniform mixture of density matrices, then $\sigma(G \otimes G')$ is separable. ∎

We associate to the vertices, $v_1, v_2, \ldots, v_n$, of a graph G an orthonormal basis $\{|v_1\rangle, |v_2\rangle, \ldots, |v_n\rangle\}$. In terms of this basis, the uw-th elements of the matrices $\sigma\left(H_{i_k j_k}\right)$ and $\sigma^{+}\left(H_{i_k j_k}\right)$ are given by $\langle v_u | \sigma\left(H_{i_k j_k}\right) | v_w\rangle$ and $\langle v_u | \sigma^{+}\left(H_{i_k j_k}\right) | v_w\rangle$, respectively. In this basis

$$\sigma\left(H_{i_k j_k}\right) = P\left[\tfrac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle - \left|v_{j_k}\right\rangle\right)\right] \quad \text{and} \quad \sigma^{+}\left(H_{i_k j_k}\right) = P\left[\tfrac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle + \left|v_{j_k}\right\rangle\right)\right].$$

Lemma 4.4. *For any $n = p \cdot q$, the density matrix $\sigma(K_n)$ is separable in $\mathbb{C}^p \otimes \mathbb{C}^q$.*

Proof. Let $v_1, v_2, \ldots, v_n$ be the vertices of K_n, with $n = p \cdot q$. Let us consider the following two orthonormal bases $\{|u_1\rangle, |u_2\rangle, \ldots, |u_p\rangle\}$ and $\{|w_1\rangle, |w_2\rangle, \ldots, |w_q\rangle\}$ of $\mathbb{C}^p$ and $\mathbb{C}^q$, respectively. For all $i = 1, 2, \ldots, n$, we then write $|v_i\rangle = |u_{s+1}\rangle |w_{s'}\rangle$, where $i = sq + s'$, $0 \le s \le p-1$ and $1 \le s' \le q$. By making use of this basis, we can write

$$\sigma(H_{i_k j_k}) = P\left[\frac{1}{\sqrt{2}}\left(|u_{s_k+1}\rangle \left|w_{s'_k}\right\rangle - |u_{t_k+1}\rangle \left|w_{t'_k}\right\rangle\right)\right],$$

where $i_k = s_k q + s'_k$, $j_k = t_k q + t'_k$, $0 \le s_k, t_k \le p-1$, and $0 \le s'_k, t'_k \le q$. By Equation (2.2),

$$\sigma(K_n) = \frac{1}{m}\sum_{k=1}^{m} P\left[\frac{1}{\sqrt{2}}\left(|u_{s_k+1}\rangle \left|w_{s'_k}\right\rangle - |u_{t_k+1}\rangle \left|w_{t'_k}\right\rangle\right)\right].$$

Since $M(K_n) = J_n - I_n$, whenever there is a term like $P\left[\frac{1}{\sqrt{2}}\left(|u_{s_k+1}\rangle \left|w_{s'_k}\right\rangle - |u_{t_k+1}\rangle \left|w_{t'_k}\right\rangle\right)\right]$ in the sum above, there is a term like $P\left[\frac{1}{\sqrt{2}}\left(|u_{s_k+1}\rangle \left|w_{t'_k}\right\rangle - |u_{t_k+1}\rangle \left|w_{s'_k}\right\rangle\right)\right]$. The uniform mixture of these two terms gives rise to the separable density matrix $\frac{1}{2}P[|u^+\rangle|w^-\rangle] + \frac{1}{2}P[|u^-\rangle|w^+\rangle]$, where $|u^\pm\rangle = \frac{1}{\sqrt{2}}\left(|u_{s_k+1}\rangle \pm |u_{t_k+1}\rangle\right)$ and $|w^\pm\rangle = \frac{1}{\sqrt{2}}\left(\left|w_{s'_k}\right\rangle \pm \left|w_{t'_k}\right\rangle\right)$. This shows that $\sigma(K_n)$ is separable. ∎

Remark 4.5. Separability of $\sigma(K_n)$ does not depend upon the labeling of $V(K_n)$. Given a graph G, an isomorphism from $V(G)$ to $V(G)$ is called *automorphism*. Under composition of maps, the set of the automorphisms of G form a group, denoted by $Aut(G)$, and called *automorphism group* of G. Note that the separability properties of G are invariant under $Aut(G)$. Since $\sigma(K_n)$ is separable, and since the automorphism group of K_n is the symmetric group S_n, $G \cong \sigma(K_n)$ is also separable.

Example 4.6. Consider the graph K_4. The vertices of K_4 are denoted by $1, 2, 3$ and 4. We associate to these vertices the orthonormal basis $\{|1\rangle = |1\rangle|1\rangle, |2\rangle = |1\rangle|2\rangle, |3\rangle = |2\rangle|1\rangle, |4\rangle = |2\rangle|2\rangle\}$. In terms of this basis, $\sigma(K_4)$ can be written as

$$\begin{aligned}
\sigma(K_4) &= \frac{1}{12}\begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix} \\
&= \frac{1}{6}P\left[|1\rangle \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)\right] + \frac{1}{6}P\left[\frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)|1\rangle\right] \\
&\quad + P\left[\frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)|2\rangle\right] + P\left[|2\rangle \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)\right] \\
&\quad + \frac{1}{3}\left\{\frac{1}{2}P\left[\frac{1}{\sqrt{2}}(|11\rangle - |22\rangle)\right] + \frac{1}{2}P\left[\frac{1}{\sqrt{2}}(|12\rangle - |21\rangle)\right]\right\}.
\end{aligned}$$

Each of the first four terms in the above expression is a projector on a product state, while the last two terms give rise to the separable density matrix $\frac{1}{2}P[|-\rangle|+\rangle] + \frac{1}{2}P[|+\rangle|-\rangle]$, where $|\pm\rangle \overset{def}{=} \frac{1}{\sqrt{2}}([|1\rangle \pm |2\rangle])$. Thus $\sigma(K_4)$ is separable in $\mathbb{C}^2 \otimes \mathbb{C}^2$.

Lemma 4.7. *The complete graph on $n > 1$ vertices is not a tensor product of graphs.*

Proof. It is clear that, if n is prime, K_n is not a tensor product of graphs. We then assume that n is not a prime. Suppose that there exist graphs G and H, respectively on p and s vertices, such that $K_{ps} = G \otimes H$. Let $|E(G)| = q$ and $|E(H)| = t$. Then, by the degree-sum formula, $2q \leq p(p-1)$ and $2t \leq s(s-1)$. So,

$$2q \cdot 2t \leq p(p-1)s(s-1) = ps(ps-p-s+1).$$

Now, observe that $|V(G \otimes H)| = ps$ and $|E(G \otimes H)| = 2(qt)$. Therefore, $G \otimes H = K_{ps}$ if and only if $ps(ps-1) = 2 \cdot 2qt$, which is true if and only if $p = s = 1$. This occurs only when $n = 1$. ∎

Theorem 4.8. *Given a graph $G \otimes H$, the density matrix $\sigma(G \otimes H)$ is separable. However if a density matrix $\sigma(L)$ is separable it does not necessarily mean that $L = G \otimes H$, for some graphs G and H.*

Proof. The theorem follows from Lemma 4.3 together with Lemma 4.4 and Lemma 4.7. ∎

Remark 4.9. Not always is $\sigma(G) \otimes \sigma(G)$ the density matrix of a graph. However, we observe the following. A *weighted graph* is a graph with each of its edges labeled by a real number. Let W be a weighted graph defined as follows: $V = \{ij' : i, j' = 1, 2\}$; the edges of W are

$$\{11', 12'\}, \{11', 21'\}, \{12', 22'\}, \{21', 22'\}, \{11', 22'\}, \{12', 21'\},$$

with weights $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$, and $-\frac{1}{2}$, respectively. We write $W := W(1,2;1',2')$. Let G be a graph on the vertices $1, 2, \ldots, n$ and the edges $\{i_1, j_1\}, \{i_2, j_2\}, \ldots, \{i_m, j_m\}$, where $1 \leq i_k, j_k \leq n$. Let H be a graph on the vertices $1', 2', \ldots, p'$ and the edges $\{s'_1, t'_1\}, \{s'_2, t'_2\}, \ldots, \{s'_q, t'_q\}$, then

$$\sigma(G) \otimes \sigma(G) = \frac{1}{mq} \sum_{k=1}^{m} \sum_{l=1}^{q} \sigma\left(i_k, j_k; s'_l, t'_l\right).$$

4.2. Stars

A *star graph* (for short, *star*) on n vertices $v_1, v_2, \ldots, v_n$, denoted by $K_{1,n-1}$, is the graph whose set of edges is $\{\{v_1, v_i\} : i = 2, 3, \ldots, n\}$. Quantum dynamics on stars has been studied in the context of quantum chaos [6].

Definition 4.10. [Entangled edge] *Let G be a graph on $n = pq$ vertices, $v_1, v_2, \ldots, v_n$. The k-th edge $\{v_{i_k}, v_{j_k}\}$ of G is identified with the pure density matrix $P\left[\frac{1}{\sqrt{2}}\left(|v_{i_k}\rangle - |v_{j_k}\rangle\right)\right]$, where $|v_{i_k}\rangle = |u_{s_k+1}\rangle|w_{t_k}\rangle$ and $|v_{j_k}\rangle = |u_{s'_k+1}\rangle|w_{t'_k}\rangle$, with $i_k = s_k q + t_k$ and $j_k = s'_k q + t'_k$, $0 \leq s_k, s'_k \leq p-1$ and $1 \leq t_k, t'_k \leq q$. The vectors $|u_i\rangle$'s and $|w_j\rangle$'s form orthonormal bases of $\mathbb{C}^p$ and $\mathbb{C}^q$, respectively. The edge $\{v_{i_k}, v_{j_k}\}$ is said to be* entangled *if $s_k \neq s'_k$ and $t_k \neq t'_k$.*

Theorem 4.11. *The density matrix $\sigma(K_{1,n-1})$ is entangled for $n = pq \geq 4$.*

Proof. Consider the graph $G = K_{1,n-1}$ on $n = p \cdot q \geq 4$ vertices, $v_1, v_2, \ldots, v_n$. Then

$$\sigma(G) = \frac{1}{n-1}\sum_{k=2}^{n}\sigma(H_{1k}) = \frac{1}{n-1}\sum_{k=2}^{n}P\left[\frac{1}{\sqrt{2}}(|v_1\rangle - |v_k\rangle)\right].$$

We are going to examine separability of $\sigma(G)$ in $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$, where $\mathbb{C}_A^p$ and $\mathbb{C}_B^q$ are associated to two quantum mechanical systems S_A and S_B, respectively. Let $\{|u_1\rangle, |u_2\rangle, \ldots, |u_p\rangle\}$ and $\{|w_1\rangle, |w_2\rangle, \ldots, |w_q\rangle\}$ be orthonormal bases of $\mathbb{C}_A^p$ and $\mathbb{C}_B^q$, respectively. So,

$$\sigma(G) = \frac{1}{n-1}\sum_{k=2}^{n}P\frac{1}{\sqrt{2}}\left[\left(|u_1\rangle|w_1\rangle - |u_{s_k+1}\rangle|w_{t_k}\rangle\right)\right],$$

where $k = s_k q + t_k$, $0 \leq s_k \leq p-1$ and $1 \leq t_k \leq q$. Thus

$$\sigma(G) = \frac{1}{n-1}\left\{\sum_{j=2}^{q}P\left[|u_1\rangle\frac{1}{\sqrt{2}}\left(|w_1\rangle - |w_j\rangle\right)\right]\right.$$
$$\left. + \sum_{i=2}^{p}P\left[\frac{1}{\sqrt{2}}(|u_1\rangle - |u_i\rangle)|w_1\rangle\right] + \sum_{j=2}^{q}\sum_{i=2}^{p}P\left[\frac{1}{\sqrt{2}}\left(|u_1\rangle|w_1\rangle - |u_i\rangle|w_j\rangle\right)\right]\right\}.$$

Consider now the following two dimensional projectors: $P = |u_1\rangle\langle u_1| + |u_2\rangle\langle u_2|$ and $Q = |w_1\rangle\langle w_1| + |w_2\rangle\langle w_2|$. Then

$$(P\otimes Q)\sigma(G)(P\otimes Q) = \frac{1}{n-1}\left\{\frac{n-4}{2}P[|u_1\rangle|w_1\rangle] + P\left[\frac{1}{\sqrt{2}}(|u_1\rangle - |u_2\rangle)|w_1\rangle\right]\right.$$
$$+ P\left[|u_1\rangle\frac{1}{\sqrt{2}}(|w_1\rangle - |w_2\rangle)\right]$$
$$\left. + P\left[\frac{1}{\sqrt{2}}(|u_1\rangle|w_1\rangle - |u_2\rangle|w_2\rangle)\right]\right\}.$$

In the basis $\{|u_1\rangle|w_1\rangle, |u_1\rangle|w_2\rangle, |u_2\rangle|w_1\rangle, |u_2\rangle|w_2\rangle\}$, we have

$$[(P\otimes Q)\sigma(G)(P\otimes Q)]^{\mathsf{T}_B} = \frac{1}{n-1}\begin{bmatrix} \frac{n-1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}. \tag{4.4}$$

The eigenvalues of the above matrix are

$$\left\{\left[\frac{1}{2(n-1)}\right], \left[\frac{1}{n-1}\right], \left[\frac{1}{4}\left(1 \pm \sqrt{(n-1)^2+8}/(n-1)\right)\right]\right\}.$$

As $n \geq 4$, $\frac{1}{4}(1 - \sqrt{(n-1)^2+8}/(n-1)) < 0$. Hence, by Criterion 4.1, the matrix $(P\otimes Q)\sigma(G)(P\otimes Q)$ is entangled and then $\sigma(G)$ is also entangled. (Note that this matrix is not normalized.) ∎

Example 4.12. Consider the graph $G = (\{1,2,3,4\}, \{\{1,2\},\{1,3\},\{1,4\},\{2,3\}\})$. We test the separability of $\sigma(G)$ in $\mathbb{C}_A^2 \otimes \mathbb{C}_B^2$, with respect to the orthonormal basis $\{|1\rangle|1\rangle, |1\rangle|2\rangle, |2\rangle|1\rangle, |2\rangle|2\rangle\}$. In this basis,

$$\sigma(G) = \frac{1}{8}\begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 2 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}.$$

It can be easily verified that $(\sigma(G))^{T_B} = \sigma(G)$. As a consequence, all the eigenvalues of $(\sigma(G))^{T_B}$ are nonnegative, as $\sigma(G)$ is positive semidefinite. It follows from Criterion 4.1 that $\sigma(G)$ is separable in $\mathbb{C}^2 \otimes \mathbb{C}^2$. Consider now the star

$$K_{1,3} = (\{1,2,3,4\}, \{\{1,2\},\{1,3\},\{1,4\}\}).$$

Observe that $K_{1,3}$ is obtained from G with the removal of the edge $\{2,3\}$. With respect to the above mentioned basis, we have

$$\sigma(K_{1,3}) = \frac{1}{6}\begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad (\sigma(K_{1,3}))^{T_B} = \frac{1}{6}\begin{bmatrix} 3 & -1 & -1 & 0 \\ -1 & 1 & -1 & 0 \\ -1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

The eigenvalues of $(\sigma(K_{1,3}))^{T_B}$ are $\frac{1}{6}$, $\frac{1}{3}$, $\frac{1}{12}\sqrt{17}+\frac{1}{4}$, and $\frac{1}{4}-\frac{1}{12}\sqrt{17}$. It follows from the Criterion 4.1 that $\sigma(K_{1,3})$ is entangled in $\mathbb{C}^2 \otimes \mathbb{C}^2$.

Remark 4.13. A density matrix ρ_{AB} acting on $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$ is said to be *distillable* if there exist a positive integer k and two 2-dimensional projectors $P_1 : \left(\mathbb{C}_A^p\right)^{\otimes k} \to \mathbb{C}^2$ and $P_2 : \left(\mathbb{C}_B^q\right)^{\otimes k} \to \mathbb{C}^2$ such that

$$\left((P_1 \otimes P_2)\,\rho_{AB}^{\otimes k}\,(P_1 \otimes P_2)\right)^{\mathsf{T}_B} \ngeq 0.$$

An entangled density matrix which is not distillable is called *bound entangled*. Theorem 4.11 actually shows that not only $\sigma(K_{1,n-1})$ is entangled but also distillable in $\mathbb{C}^p \otimes \mathbb{C}^q$ where $n = pq \geq 4$.

Second proof of Theorem 4.11. Let G be a graph on n vertices and m edges. Suppose that G has l_i loops at the vertex v_i. Then $|E(G)| = m + \sum_{i=1}^n l_i$ edges. We associate to G the following density matrix

$$\sigma_\circ(G) \stackrel{def}{=} \left(2m + \sum_{i=1}^n l_i\right)^{-1} (\Delta(G) - M(G)) + \left(2m + \sum_{i=1}^n l_i\right)^{-1} \Delta_\circ(G), \qquad (4.5)$$

where $\Delta_\circ(G) = \bigoplus_{i=1}^n l_i P[|v_i\rangle]$.

The matrix $\sigma_\circ(G)$ generalizes the notion of density matrix of a graph by taking into account loops. The star $K_{1,3}$ is called a *claw*. We denote by $K_{1,3}^{+l}$ a claw with l loops at the vertex of degree 3. In order to prove the theorem, we first show that $K_{1,3}^{+l}$ is entangled in $\mathbb{C}_A^2 \otimes \mathbb{C}_B^2$. The vertices of $K_{1,3}$ are denoted by $u_1w_1, u_1w_2, u_2w_1, u_2w_2$, where $d(u_1w_1) = 3$. Then we have

$$\sigma_\circ\left(K_{1,3}^{+l}\right) = \frac{2}{l+6}\left\{\frac{l}{2}P\left[|u_1\rangle|w_1\rangle\right] + P\left[\frac{1}{\sqrt{2}}(|u_1\rangle|w_1\rangle - |u_2\rangle|w_2\rangle)\right]\right.$$
$$\left. + P\left[\frac{1}{\sqrt{2}}(|u_1\rangle - |u_2\rangle|w_1\rangle)\right] + P\left[|u_1\rangle\frac{1}{\sqrt{2}}(|w_1\rangle - |w_2\rangle)\right]\right\}.$$

One can check that $\left[\sigma_\circ\left(K_{1,3}^{+l}\right)\right]^{\intercal_B} \ngeq 0$. By Theorem 4.1, $\sigma_\circ\left(K_{1,3}^{+l}\right)$ is entangled in $\mathbb{C}_A^2 \otimes \mathbb{C}_B^2$, for all $l \geq 0$. Let A be the matrix in Equation (4.4). Taking $n-4 = l$, $A = \frac{l+6}{2(l+3)}\sigma_\circ\left(K_{1,3}^{+l}\right)$. Then A is entangled in $\mathbb{C}_A^2 \otimes \mathbb{C}_B^2$. This shows that $\sigma(K_{1,n-1})$ is entangled in $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$. ∎

Proposition 4.14. *Separability of* $\sigma(K_{1,n-1})$*, with* $n = pq \geq 4$*, does not depend on the labeling of* $V(K_{1,n-1})$.

Proof. In $K_{1,n-1}$, the vertex of degree $(n-1)$ is called *root*, the other vertices are called *leaves*. We define two types of isomorphisms for stars: *Leaf-shuffling*. An isomorphism ι acting on $V(K_{1,n-1})$ is called a *leaf-shuffling* if $\iota(r) = r$, where r is the root of $K_{1,n-1}$; *Root-swapping*. An isomorphism ι acting on $V(K_{1,n-1})$ is called a *root-swapping* if $\iota(r) = v$, where r is the root of $K_{1,n-1}$ and v is a leaf. All graphs in the isomorphism class of $K_{1,n-1}$ can be obtained by combining leaf-shuffling and root-swapping. It is clear that leaf-shuffling is an automorphism and hence it does not change the separability property of $\sigma(K_{1,n-1})$. We now prove that this is the case also for root-swapping. We label the vertices of a graph $G \cong K_{1,n-1}$ as $u_1w_1, u_1w_2, \ldots, u_1w_q, u_2w_1, u_2w_2, \ldots, u_2w_q, \ldots, u_pw_q$. Let u_1w_1 be the root of G and let $\iota\colon V(G) \to V(H)$ be a root-swapping. Then, the root of H is $\iota(u_1w_1) = u_iw_j$, where $(1,1) \neq (i,j)$. Denote by $P_{1\leftrightarrow i}$ and $Q_{1\leftrightarrow j}$ the permutation matrices defined as follows: $P_{1\leftrightarrow i}|u_1\rangle = |u_i\rangle$ and $P_{1\leftrightarrow i}|u_{i'}\rangle = |u_{i'}\rangle$, for $i' \neq 1$; $Q_{1\leftrightarrow j}|w_1\rangle = |w_j\rangle$ and $Q_{1\leftrightarrow j}|w_{j'}\rangle = |w_{j'}\rangle$, for $j' \neq 1$. Then we have $(P_{1\leftrightarrow i} \otimes Q_{1\leftrightarrow j})\,\sigma(G)\,(P_{1\leftrightarrow i} \otimes Q_{1\leftrightarrow j})^\intercal = \sigma(H)$. Then $\sigma(G)$ is entangled if and only if $\sigma(H)$ is entangled. ∎

Remark 4.15. For $K_{1,n-1}$, with $n = pq \geq 4$, $K_{1,n-1} \ncong G \otimes H$, where $|V(G)| = p$ and $|V(H)| = q$.

4.3. Perfect Matchings

A *matching* of a graph is a set of vertex-disjoint edges. A *perfect matching* of a graph G is a matching spanning $V(G)$.

Definition 4.16. [e-matching; pe-matching] *An* e-matching *is a matching having all edges entangled. Each vertex of an e-matching on* $n = pq$ *vertices can be labeled by an ordered pair* (i, j)*, where* $1 \leq i \leq p$ *and* $1 \leq j \leq q$*. A* pe-matching *of a graph* G *is an e-matching spanning* $V(G)$.

Theorem 4.17. *Let G be a graph on $n = 2p$ vertices. If all the entangled edges of G belong to the same pe-matching then $\sigma(G)$ is separable in $\mathbb{C}^2 \otimes \mathbb{C}^p$.*

Our proof of the theorem involves the use of the following concepts.

Definition 4.18. [Criss-cross] *A* criss-cross *is a set $\{\{(k,i),(l,j)\},\{(k,j),(l,i)\}\}$ of two edges belonging to an e-matching on $n = pq$ vertices.*

Definition 4.19. [Tally-mark] *A set*

$$\{(k,i_1),(l,i_2)\},\{(k,i_2),(l,i_3)\},\ldots,\{(k,i_{s+1}),(l,i_{s+2})\},\{(k,i_{s+2}),(l,i_1)\}$$

of $s+2$ edges, where $k < l$, $s \geq 0$ and $i_1 < i_2 < \cdots < i_{s+2}$, belonging to an e-matching on $n = pq$ vertices, is called a tally-mark. (*Note that a criss-cross is a tally-mark with two edges.*)

Definition 4.20. [Canonical pe-matching] *Let H be an e-matching on $n = pq$ vertices. Then H is said to be* canonical *if $H = H_1 \uplus H_2 \uplus \cdots \uplus H_k$, where every graph $H_1, H_2, \ldots, H_k$ is a tally-mark.*

Lemma 4.21. *From any pe-matching H on $n = 2p$ vertices, labeled by (i, j), where $i = 1,2$ and $1 \leq j \leq p$, we can always obtain a canonical pe-matching by applying a permutation to the second label of all the vertices of H.*

Proof. Let H be a pe-matching as in the statement of the lemma. Any pe-matching can be taken as a set of criss-crosses and e-matchings, the latter being of the forms:

- H_1 such that $E(H_1) = \{\{(1,i_1),(2,j_1)\},\{(1,i_2),(2,j_2)\},\ldots,\{(1,i_k),(2,j_k)\}\}$, where $\{i_1,i_2,\ldots,i_k\} = \{j_1,j_2,\ldots,j_k\}$;
- H_2 such that $E(H_2) = \{\{(1,i'_1),(2,j'_1)\},\{(1,i'_2),(2,j'_2)\},\ldots,\{(1,i'_l),(2,j'_l)\}\}$, where $\{i'_1,i'_2,\ldots,i'_l\} = \{j'_1,j'_2,\ldots,j'_l\}$ and $\{i_1,i_2,\ldots,i_k\} \cap \{i'_1,i'_2,\ldots,i'_l\} = \emptyset$;
- $\cdots$.

We describe an algorithm to obtain a tally-mark from any of the above e-matchings. It is sufficient to describe the algorithm for H_1. Without loss of generality we take $i_1 < i_2 < \cdots < i_k$. We permute the 2^{nd} labels of the edges of H_1, to form one or more disjoint tally-marks. Consider the s-th step in the construction: if $j_s < i_s$, we have completed a tally-mark; if $j_s > i_s$, then we perform a permutation on the 2^{nd} label of a vertex $(\cdot, i)$ acting on indices $i > i_s$, which maps the edge $\{(1,i_s),(2,j_s)\}$ to the edge $\{(1,i_s),(2,i_{s+1})\}$ (adding another downstroke to a tally-mark, yet incomplete). It is easy to see that applying this rule successively to the labels $\{i_1,i_2,\ldots,i_k\}$, in ascending order, produces a set of one or more disjoint tally-marks. ∎

Example 4.22. In Figure 1, a pe-matching (top graph) is transformed in a canonical pe-matching by applying a permutation on the second labels of the vertices. We first apply the permutation $(2\,3)$ (central graph). We then apply the permutation $(3\,5)$ (bottom graph).

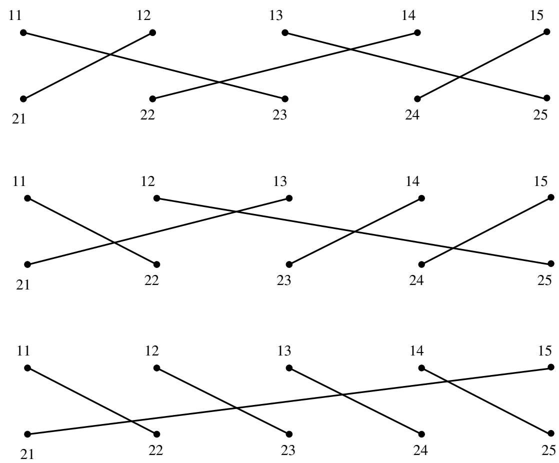


Figure 1.

Lemma 4.23. *Let H be a tally-mark on $n = 2k+2$ vertices. Then $\sigma(H)$ is separable in $\mathbb{C}^2 \otimes \mathbb{C}^{k+1}$.*

Proof. Let H be a tally-mark. Let us assume that H is not a criss-cross. In fact, if H is a criss-cross then $\sigma(H)$ is obviously separable in $\mathbb{C}^2 \otimes \mathbb{C}^2$. Let

$$E(H) = \{\{(1,i_0),(2,i_1)\},\{(1,i_1),(2,i_2)\},\ldots,\{(1,i_{k-1}),(2,i_k)\},\{(1,i_k),(2,i_0)\}\},$$

where $i_0 < i_1 < \cdots < i_k$. We associate the vector $|l\rangle|i_s\rangle$ to the vertex $(l,i_s) \in V(H)$, where $l = 1,2$ and $s = 0,1,2,\ldots,k$. Then

$$\sigma(H) = \frac{1}{k+1}\sum_{s=0}^{k} P\left[\frac{1}{\sqrt{2}}\left(|1\rangle|i_s\rangle - |2\rangle\left|i_{(s+1)\,\mathrm{mod}(k+1)}\right\rangle\right)\right].$$

Let us consider the permutation g on the $(k+1)$ letters $i_0,i_1,\ldots,i_k$ defined as follows: $g\colon i_s \mapsto i_{(s+1)\,\mathrm{mod}(k+1)}$, where $0 \le s \le k$. The order of g is then $(k+1)$. Let $\Gamma = \langle g\rangle \cong \mathbb{Z}_{k+1}$ and $\rho_{reg}(g) = \Pi$. One can check that

$$\sigma(H) = \frac{1}{k+1}\sum_{s=0}^{k}(I_2\otimes\Pi^s)\,P\left[\frac{1}{\sqrt{2}}\left(|1\rangle|i_0\rangle - |2\rangle|i_1\rangle\right)\right]\left(I_2\otimes\Pi^{k+1-s}\right), \tag{4.6}$$

where I_2 acts on the Hilbert space spanned by the vectors $|1\rangle$ and $|2\rangle$. We are now looking for the density matrices acting on $\mathbb{C}^2\otimes\mathbb{C}^{k+1}$, which remain invariant under the action of Γ. Let

$$|\psi_m\rangle = \frac{1}{\sqrt{k+1}}\sum_{s=0}^{k}\exp\left[\frac{2\pi i s m}{k+1}\right]|i_s\rangle, \quad \text{where } m = 0,1,2,\ldots,k.$$

Observe that the vectors $|\psi_m\rangle$'s are pairwise orthonormal. Then $\Pi^l|\psi_m\rangle = \exp\left[\frac{2\pi ilm}{k+1}\right]|\psi_m\rangle$, for $l = 0, 1, 2, \ldots, k$ and $m = 0, 1, 2, \ldots, k$. It follows that the $|\psi_m\rangle$'s are eigenvectors of Π^l. Let

$$|\Psi\rangle = \sum_{m=0}^{k} (\alpha_m|1\rangle + \beta_m|2\rangle)\,|\psi_m\rangle, \quad \text{where} \sum_{m=0}^{k} \left(|\alpha_m|^2 + |\beta_m|^2\right) = 1,$$

be a vector in $\mathbb{C}^2 \otimes \mathbb{C}^{k+1}$. Then

$$\left(I_2 \otimes \Pi^l\right)|\Psi\rangle\langle\Psi|\left(I_2 \otimes \Pi^{k+1-l}\right) = |\Psi\rangle\langle\Psi|,$$

where $l = 0, 1, 2, \ldots, k$, if and only if $|\Psi\rangle$ is one of the forms $(\alpha_m|1\rangle + \beta_m|2\rangle)|\psi_m\rangle$, for $m = 0, 1, 2, \ldots, k$. This shows that, for any density matrix ρ acting on $\mathbb{C}^2 \otimes \mathbb{C}^{k+1}$, the following density matrix

$$\rho' = \frac{1}{k+1}\sum_{s=0}^{k} (I_2 \otimes \Pi^s)\,\rho\left(I_2 \otimes \Pi^{k+1-s}\right)$$

is a mixture of all the projectors $P\left[\frac{1}{\sqrt{2}}(\alpha_m|1\rangle + \beta_m|2\rangle)\,|\psi_m\rangle\right]$, where $m = 0, 1, 2, \ldots, k$. Hence ρ' is separable. By Equation (4.6), $\sigma(H)$ is also separable:

$$\sigma(H) = \frac{1}{k+1}\sum_{m=0}^{k} P\left[\frac{1}{\sqrt{2}}\left(|1\rangle - \exp\left[-\tfrac{2\pi im}{k+1}\right]|2\rangle\right)|\psi_m\rangle\right]. \qquad \blacksquare$$

Given a graph G and a factor H of G, we denote by $G\backslash H$ the graph with adjacency matrix $M(G\backslash H) \overset{def}{=} M(G) - M(H)$.

Proof of Theorem 4.17. Let G be as in the statement of the theorem. In addition, we assume that $|E(G)| = m$. Let H be the pe-matching containing all the entangled edges of G. Then $\sigma(G) = \frac{p}{m}\sigma(H) + \frac{m-p}{m}\sigma(G\backslash H)$. The density matrix $\sigma(G\backslash H)$ is separable by assumption. Lemma 4.21 together with Lemma 4.23 shows that $\sigma(H)$ is separable in $\mathbb{C}^2 \otimes \mathbb{C}^p$. This proves the theorem. $\blacksquare$

Theorem 4.24. *The pe-matching in* Figure 2 *is separable in* $\mathbb{C}^3 \otimes \mathbb{C}^4$.

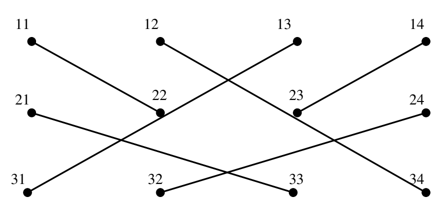


Figure 2.

Proof. Let G be the pe-matching in the figure. Then $\sigma(G) = \frac{1}{6}\sum_{i=1}^{6} P[|\psi_i^-\rangle]$, where $|\psi_1^\pm\rangle = \frac{1}{\sqrt{2}}(|1\rangle|1\rangle \pm |2\rangle|2\rangle)$, $|\psi_2^\pm\rangle = \frac{1}{\sqrt{2}}(|1\rangle|4\rangle \pm |2\rangle|3\rangle)$, $|\psi_3^\pm\rangle = \frac{1}{\sqrt{2}}(|1\rangle|2\rangle \pm |3\rangle|4\rangle)$,

$|\psi_4^{\pm}\rangle = \frac{1}{\sqrt{2}}(|1\rangle|3\rangle \pm |3\rangle|1\rangle)$, $|\psi_5^{\pm}\rangle = \frac{1}{\sqrt{2}}(|2\rangle|1\rangle \pm |3\rangle|3\rangle)$ and $|\psi_6^{\pm}\rangle = \frac{1}{\sqrt{2}}(|2\rangle|4\rangle \pm |3\rangle|2\rangle)$. Here $(\sigma(G))^{\intercal_B} = (I_3 \otimes P)\sigma(G)(I_3 \otimes P^{\intercal})$, where

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

Then $(\sigma(G))^{\intercal_B} \geq 0$. Since a density matrix having positive partial transpose is either separable or bound entangled [4], this holds for $\sigma(G)$. We are now going to show that $\sigma(G)$ is separable in $\mathbb{C}^3 \otimes \mathbb{C}^4$. Let $|\chi\rangle$ be in the support of $\sigma(G)$. Then $|\chi\rangle = \sum_{i=1}^{6} a_i|\psi_i^-\rangle = \frac{1}{\sqrt{2}}|1\rangle(a_1|1\rangle + a_3|2\rangle + a_4|3\rangle + a_2|4\rangle) + \frac{1}{\sqrt{2}}|2\rangle(a_5|1\rangle - a_1|2\rangle - a_2|3\rangle + a_6|4\rangle) - \frac{1}{\sqrt{2}}|3\rangle(a_4|1\rangle + a_6|2\rangle + a_5|3\rangle + a_3|4\rangle)$. So, $|\chi\rangle$ is separable if and only if $(a_1, a_3, a_4, a_2) = \lambda(a_5, -a_1, -a_2, a_6) = \mu(a_4, a_6, a_5, a_3)$, where $\lambda, \mu \in \mathbb{C}$. Then

$$a_1 = \lambda a_5 = \mu a_4,\ a_3 = -\lambda a_1 = \mu a_6,\ a_4 = -\lambda a_2 = \mu a_5,\ a_2 = \lambda a_6 = \mu a_3, \qquad (4.7)$$

where $\lambda \neq 0$. In fact, if $\lambda = 0$ and $\mu \neq 0$, then $a_i = 0$ for $i = 1, 2, \ldots, 6$, which is impossible. On the other hand, if $\lambda = \mu = 0$ then $a_1, a_2, a_3, a_4 = 0$. Then $|\chi\rangle = \frac{1}{\sqrt{2}}|2\rangle(a_5|1\rangle + a_6|4\rangle) - \frac{1}{\sqrt{2}}|3\rangle(a_6|2\rangle + a_5|3\rangle)$, which is entangled as $|a_5|^2 + |a_6|^2 \neq 0$. Similarly, it can be shown that $\mu \neq 0$. Therefore, from Equation (4.7), $\lambda^3 = 1$ and $\mu^2 = \lambda$, and we can distinguish the following cases.

Case 1. $(\lambda = \mu = 1)$ We have $a_2 = a_3 = a_6 = -a_1$ and $a_4 = a_5 = a_1$. So $|\chi\rangle = \frac{a_1}{\sqrt{2}}(|1\rangle + |2\rangle - |3\rangle)(|1\rangle - |2\rangle + |3\rangle - |4\rangle)$.

Case 2. $(\lambda = 1, \mu = -1)$ We have $a_2 = a_5 = a_6 = a_1$ and $a_3 = a_4 = -a_1$. So $|\chi\rangle = \frac{a_1}{\sqrt{2}}(|1\rangle + |2\rangle + |3\rangle)(|1\rangle - |2\rangle - |3\rangle + |4\rangle)$.

Case 3. $\left(\lambda = \omega = e^{2\pi i/3}, \mu = -\omega^2\right)$ We have $a_2 = a_1, a_3 = a_4 = -\omega a_1, a_5 = a_6 = \omega^2 a_1$. So $|\chi\rangle = \frac{a_1}{\sqrt{2}}\left(|1\rangle + \omega^2|2\rangle + \omega|3\rangle\right)(|1\rangle - \omega|2\rangle - \omega|3\rangle + |4\rangle)$.

Case 4. $\left(\lambda = \omega, \mu = \omega^2\right)$ We have $a_2 = -a_1, a_3 = -a_4 = -\omega a_1, a_5 = -a_6 = \omega^2 a_1$. So $|\chi\rangle = \frac{a_1}{\sqrt{2}}\left(|1\rangle + \omega^2|2\rangle - \omega|3\rangle\right)(|1\rangle - \omega|2\rangle + \omega|3\rangle - |4\rangle)$.

Case 5. $\left(\lambda = \omega^2, \mu = \omega\right)$ We have $a_2 = -a_1, a_3 = -a_4 = -\omega^2 a_1, a_5 = -a_6 = \omega a_1$. So $|\chi\rangle = \frac{a_1}{\sqrt{2}}\left(|1\rangle + \omega|2\rangle - \omega^2|3\rangle\right)\left(|1\rangle - \omega^2|2\rangle + \omega^2|3\rangle - |4\rangle\right)$.

Case 6. $\left(\lambda = \omega^2, \mu = -\omega\right)$ We have $a_2 = a_1$, $a_3 = a_4 = -\omega^2 a_1$, $a_5 = a_6 = \omega a_1$. So $|\chi\rangle = \frac{a_1}{\sqrt{2}}\left(|1\rangle + \omega|2\rangle + \omega^2|3\rangle\right)\left(|1\rangle - \omega^2|2\rangle - \omega^2|3\rangle + |4\rangle\right)$.

Thus we can observe that the range of the rank six density matrix $\sigma(G)$ contains only the following six separable states: $|\chi_1\rangle = \frac{1}{\sqrt{3}}(|1\rangle + |2\rangle - |3\rangle)\frac{1}{2}(|1\rangle - |2\rangle + |3\rangle - |4\rangle)$, $|\chi_2\rangle = \frac{1}{\sqrt{3}}(|1\rangle + |2\rangle + |3\rangle)\frac{1}{2}(|1\rangle - |2\rangle - |3\rangle + |4\rangle)$, $|\chi_3\rangle = \frac{1}{\sqrt{3}}(|1\rangle + \omega^2|2\rangle + \omega|3\rangle)\frac{1}{2}(|1\rangle - \omega|2\rangle - \omega|3\rangle + |4\rangle)$, $|\chi\rangle = \frac{1}{\sqrt{3}}(|1\rangle + \omega^2|2\rangle - \omega|3\rangle)\frac{1}{2}(|1\rangle - \omega|2\rangle + \omega|3\rangle - |4\rangle)$, $|\chi_5\rangle = \frac{1}{\sqrt{3}}(|1\rangle + \omega|2\rangle - \omega^2|3\rangle)\frac{1}{2}(|1\rangle - \omega^2|2\rangle + \omega^2|3\rangle - |4\rangle)$ and $|\chi_6\rangle = \frac{1}{\sqrt{3}}(|1\rangle + \omega|2\rangle + \omega^2|3\rangle)$

$\frac{1}{2}(|1\rangle - \omega^2|2\rangle - \omega^2|3\rangle + |4\rangle)$. These states are pairwise orthogonal. As $\sigma(G)$ is proportional to a six dimensional projector, we can write $\sigma(G) = \frac{1}{6}\sum_{i=1}^{6} |\chi_i\rangle\langle\chi_i|$, and hence $\sigma(G)$ is separable. ∎

Remark 4.25. The pe-matching G in Figure 3 is entangled in $\mathbb{C}^3 \otimes \mathbb{C}^4$. In fact, it can be shown that $(\sigma(G))^{T_B} \ngeq 0$.

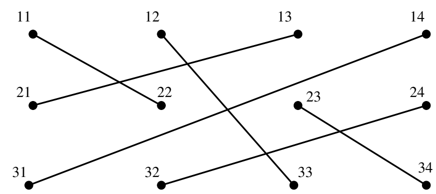


Figure 3.

4.4. The Petersen Graph

Let v, k and i be fixed positive integers, with $v \geq k \geq i$. Let S be an n-elements set. The *Johnson graph* $J(v, k, i)$ is defined as follows: the vertices of $J(v, k, i)$ are the k-elements subsets of S; two vertices are adjacent if their intersection has size i. The graph $J(5, 2, 0)$ is called *Petersen graph* and it has a number of important properties. For example, it is strongly-regular and transitive. A graph G that is not complete is said to be *strongly-regular* if it is regular, every pair of adjacent vertices has the same number of common neighbours, and every pair of nonadjacent vertices has the same number of common neighbours. A graph G is said to be *transitive* if $Aut(G)$ acts transitively on $V(G)$. A permutation group Γ *acts transitively* on a set S if, for any $s, t \in S$, there exists $g \in \Gamma$, such that $g(s) = t$.

Theorem 4.26. *Let G be a Petersen graph. Then* $\sigma(G)$ *is either separable or entangled in* $\mathbb{C}^2 \otimes \mathbb{C}^5$*, depending on the labelling of G.*

Proof. Let G (left) and H (right) be the graphs in Figure 4:

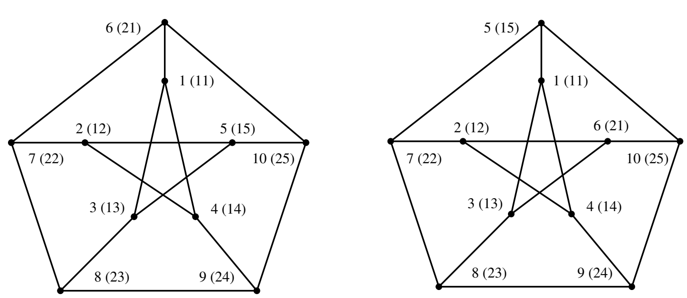


Figure 4.

Both G and H are isomorphic to the Petersen graph. The density matrix $\sigma(G)$ is separable, since every edge of G is separable. The density matrix of H is entangled in $\mathbb{C}_A^2 \otimes \mathbb{C}_B^5$, since it can be shown that $(\sigma(H))^{\mathsf{T}_B} \ngeq 0$. ∎

Corollary 4.27. *The density matrices of strongly-regular graphs and transitive graphs can be separable or entangled.*

Proof. By Theorem 4.26, since the Petersen graph is strongly-regular and transitive. ∎

4.5. Concurrence

Let $|\psi\rangle_{AB} \in \mathbb{C}_A^2 \otimes \mathbb{C}_B^2$. The notion of concurrence was introduced by Wootters [12]. The *concurrence* of $|\psi\rangle_{AB}$ is denoted and defined as follows:

$$\mathcal{C}(\psi) = \sqrt{2\left(1 - \operatorname{tr}\left(\rho_A^2\right)\right)},$$

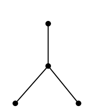
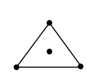
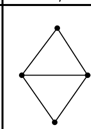
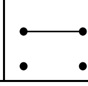
where $\rho_A = \operatorname{tr}_B(|\psi\rangle_{AB}\langle\psi|)$. Let ρ_{AB} be a density matrix acting on $\mathbb{C}_A^2 \otimes \mathbb{C}_B^2$. The concurrence of ρ_{AB} is denoted and defined as follows:

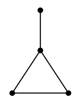
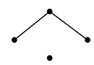
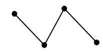
$$\mathcal{C}(\rho_{AB}) = \inf\left\{\sum_i \omega_i \mathcal{C}(\psi_i) : \rho_{AB} = \sum_i \omega_i |\psi_i\rangle_{AB}\langle\psi_i|\right\},$$

where $0 \leq \omega_i \leq 1, \sum_i \omega_i = 1$. Let $\sigma_y = -i|1\rangle\langle 2| + i|2\rangle\langle 1|$, where $|1\rangle$ and $|2\rangle$ are the eigenvectors of the matrix

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

corresponding to the eigenvalues 1 and -1, respectively. Let M^* be the conjugate of a complex matrix M. An analytical formula for $\mathcal{C}(\rho_{AB})$, is given by $\mathcal{C}(\rho_{AB}) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$, where λ_1, λ_2, λ_3 and λ_4 are the square roots of the eigenvalues of $\rho_{AB}\widetilde{\rho}_{AB}$ arranged in decreasing order, and $\widetilde{\rho}_{AB} := (\sigma_y \otimes \sigma_y)\rho_{AB}^*(\sigma_y \otimes \sigma_y)$. There are 12 nonisomorphic graphs on 4 vertices. Seven of these graphs have entangled density matrices, independently of the labeling. In the table below, the graphs and the respective concurrence are given. Note that in these cases the value of the concurrence is exactly fractional.

Concurrence	$1/3$	$1/3$	$1/5$	1
Graph				

Concurrence	1/4	1/2	1/3
Graph			

5. Graph Operations

A *graph operation* is a map that takes a graph to another one. In graph theory, the study of graph operations consists of a vast literature [10]. The following are two examples of graph operations.

Example 5.1. Deleting an edge $\{v_i, v_j\}$ from a graph G means to transform G into the graph $G - \{v_i, v_j\} \stackrel{def}{=} (V(G), E(G) \backslash \{v_i, v_j\})$. *Adding an edge* $\{v_i, v_j\}$ to a graph G, where $\{v_i, v_j\} \notin E(G)$, means to transform G into the graph $G + \{v_i, v_j\} \stackrel{def}{=} (V(G), E(G) \cup \{v_i, v_j\})$. *Deleting a vertex* v_i from a graph G means to transform G into the graph $G - v_i \stackrel{def}{=} (V(G) \backslash \{v_i\}, E(G) \backslash E_i)$, where E_i is the set of all edges incident to v_i. *Adding a vertex* v_i to a graph G means to transform G into the graph $G + v_i + T_i \stackrel{def}{=} (V(G) \cup \{v_i\}, E(G) \cup T_i)$, where T_i is an arbitrary set of edges incident to v_i.

Let $\mathcal{B}(\mathcal{H}^n)$ be the space of all bounded linear operators on $\mathcal{H}^n$. A linear map $\Lambda\colon \mathcal{B}(\mathcal{H}^n) \to \mathcal{B}(\mathcal{H}^m)$ is said to be *hermiticity preserving* if for every Hermitian operator $O \in \mathcal{B}(\mathcal{H}^n)$, $\Lambda(O)$ is an hermitian operator in $\mathcal{B}(\mathcal{H}^m)$. A hermiticity preserving map $\Lambda\colon \mathcal{B}(\mathcal{H}^n) \to \mathcal{B}(\mathcal{H}^m)$ is said to be *positive* if for any positive operator $O \in \mathcal{B}(\mathcal{H}^n)$, $\Lambda(O)$ is a positive operator in $\mathcal{B}(\mathcal{H}^m)$. A positive map $\Lambda\colon \mathcal{B}(\mathcal{H}^n) \to \mathcal{B}(\mathcal{H}^m)$ is said to be *completely positive* if for each positive integer k, $(\Lambda \otimes I_{k^2})\colon \mathcal{B}(\mathcal{H}^n \otimes \mathcal{H}^k) \to \mathcal{B}(\mathcal{H}^m \otimes \mathcal{H}^k)$ is again a positive map. A completely positive map $\Lambda\colon \mathcal{B}(\mathcal{H}^n) \to \mathcal{B}(\mathcal{H}^m)$ is said to be *trace preserving* if $\mathrm{tr}(\Lambda(O)) = \mathrm{tr}(O)$, for all $O \in \mathcal{B}(\mathcal{H}^n)$. A *quantum operation* is a trace preserving completely positive map (for short, TPCP). In standard quantum mechanics, any physical transformation of a quantum mechanical system is described by a quantum operation. We are going to use the following result:

Theorem 5.2. [Kraus Representation Theorem] *Given a quantum operation* $\Lambda\colon \mathcal{B}(\mathcal{H}^n) \to \mathcal{B}(\mathcal{H}^m)$*, there exist* $n \times m$ *matrices* A_i*, such that* $\Lambda(\rho) = \sum_i A_i \rho A_i^\dagger$*, where* ρ *is any density matrix acting on* $\mathcal{H}^n$ *and* $\sum_i A_i^\dagger A_i = I_m$*.* (*The converse is also true.*) *The matrices* A_i*'s are called* Kraus operators*.*

A *projective measurement* $\mathcal{M} = \{P_i\colon i = 1, 2, \ldots, n\}$, on a quantum mechanical system S whose state is ρ, consists of pairwise orthogonal projectors $P_i\colon \mathcal{H}_S \to \mathcal{H}_S$, such that $\sum_{i=1}^n P_i = I_{\dim(\mathcal{H}_S)}$. The i-th outcome of the measurement occurs with probability $\mathrm{tr}(P_i \rho)$ and the post-measurement state of S is $(P_i \rho P_i)/\mathrm{tr}(P_i \rho)$. Whenever the i-th outcome of the measurement occurs, we say that P_i *clicks*.

5.1. Deleting and Adding an Edge

Here we describe how to delete or add an edge by means of TPCP. Let G be a graph on n vertices, $v_1, v_2, \ldots, v_n$, and m edges, $\{v_{i_1}, v_{j_1}\}, \{v_{i_2}, v_{j_2}\}, \ldots, \{v_{i_m}, v_{j_m}\}$, where $1 \leq i_1, j_1, i_2, j_2, \ldots, i_m, j_m \leq n$. Our purpose is to delete the edge $\{v_{i_k}, v_{j_k}\}$. Then we have

$$\sigma(G) = \frac{1}{m}\sum_{l=1}^{m} \sigma(H_{i_l j_l}) = \frac{1}{m}\sum_{l=1}^{m} P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_l}\right\rangle - \left|v_{j_l}\right\rangle\right)\right]$$

and

$$\sigma\left(G - \{v_{i_k}, v_{j_k}\}\right) = \frac{1}{m-1}\sum_{\substack{l=1\\ l\neq k}}^{m} \sigma(H_{i_l j_l}) = \frac{1}{m-1}\sum_{\substack{l=1\\ l\neq k}}^{m} P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_l}\right\rangle - \left|v_{j_l}\right\rangle\right)\right].$$

A measurement in the following basis, $\mathcal{M} = \left\{\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle \pm \left|v_{j_k}\right\rangle\right), |v_i\rangle : i \neq i_k, j_k \text{ and } i = 1, 2, \ldots, n\right\}$ is performed on the system prepared in the state $\sigma(G)$. The probability that $P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle + \left|v_{j_k}\right\rangle\right)\right]$ clicks is

$$\begin{aligned} &\frac{m-1}{2m}\left(\langle v_{i_k}| + \langle v_{j_k}|\right)\sigma\left(G - \left\{v_{i_k}, v_{j_k}\right\}\right)\left(\left|v_{i_k}\right\rangle + \left|v_{j_k}\right\rangle\right) \\ &\quad = \frac{1}{4m}\sum_{\substack{l=1\\ l\neq k}}^{m}\left(\delta_{i_k i_l} - \delta_{i_k j_l} + \delta_{j_k i_l} - \delta_{j_k j_l}\right)^2. \end{aligned} \tag{5.1}$$

The state after the measurement is $P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_l}\right\rangle + \left|v_{j_l}\right\rangle\right)\right]$. Let U_{kl}^{+} be an $n \times n$ unitary matrix, such that $U_{kl}^{+}\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle + \left|v_{j_k}\right\rangle\right) = \frac{1}{\sqrt{2}}\left(\left|v_{i_l}\right\rangle - \left|v_{j_l}\right\rangle\right)$, for $l = 1, 2, \ldots, k-1, k+1, \ldots, m$. Now, with probability $1/(m-1)$ we apply U_{kl}^{+} on $P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle + \left|v_{j_k}\right\rangle\right)\right]$, for each $l = 1, 2, \ldots, k-1, k+1, \ldots, m$. Finally we obtain $\sigma\left(G - \{v_{i_k}, v_{j_k}\}\right)$ with probability given by Equation (5.1). The probability that $P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle - \left|v_{j_k}\right\rangle\right)\right]$ clicks is

$$\frac{1}{4m}\sum_{l=1}^{m}\left(\delta_{i_k i_l} - \delta_{i_k j_l} - \delta_{j_k i_l} + \delta_{j_k j_l}\right)^2. \tag{5.2}$$

The state after the measurement is $P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_l}\right\rangle - \left|v_{j_l}\right\rangle\right)\right]$. Let U_{kl}^{-} be an $n \times n$ unitary matrix, such that $U_{kl}^{-}\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle - \left|v_{j_k}\right\rangle\right) = \frac{1}{\sqrt{2}}\left(\left|v_{i_l}\right\rangle - \left|v_{j_l}\right\rangle\right)$, for $l = 1, 2, \ldots, k-1, k+1, \ldots, m$. With probability $1/(m-1)$ we apply U_{kl}^{-} on $P[\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle - \left|v_{j_k}\right\rangle\right)]$, for each $l = 1, 2, \ldots, k-1, k+1, \ldots, m$. Finally, we obtain $\sigma\left(G - \left\{v_{i_k}, v_{j_k}\right\}\right)$ with probability given by Equation (5.2). The probability that $P[|v_i\rangle]$, where $i \neq i_k, j_k$ and $i = 1, 2, \ldots, n$, clicks is

$$\frac{1}{2m}\sum_{l=1}^{m}\left(\delta_{i i_l} - \delta_{i j_l}\right)^2 \tag{5.3}$$

and the state after the measurement is $P[|v_i\rangle]$. Let U_{il} be an $n \times n$ unitary matrix, such that $U_{il}|v_i\rangle = \frac{1}{\sqrt{2}}\left(\left|v_{i_l}\right\rangle - \left|v_{j_l}\right\rangle\right)$, for $l = 1, 2, \ldots, k-1, k+1, \ldots, m$. With probability

$1/(m-1)$ we apply U_{il} on $P[|v_i\rangle]$, for each $l = 1, 2, \ldots, k-1, k+1, \ldots, m$. We obtain $\sigma\left(G - \left\{v_{i_k}, v_{j_k}\right\}\right)$ with probability given by Equation (5.3). This completes the process. The set of Kraus operators that realize the TPCP for deleting the edge $\left\{v_{i_k}, v_{j_k}\right\}$ is then

$$\left\{\frac{1}{\sqrt{m-1}}U_{kl}^{+}P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle + \left|v_{j_k}\right\rangle\right)\right] : l = 1, 2, \ldots, k-1, k+1, \ldots, m\right\}$$
$$\bigcup\left\{\frac{1}{\sqrt{m-1}}U_{kl}^{-}P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle - \left|v_{j_k}\right\rangle\right)\right] : l = 1, 2, \ldots, k-1, k+1, \ldots, m\right\}$$
$$\bigcup\left\{\frac{1}{\sqrt{m-1}}U_{il}P[|v_i\rangle] : i = 1, 2, \ldots, n;\ i \neq i_k, j_k;\ l = 1, 2, \ldots, k-1, k+1, \ldots, m\right\}.$$

The set of Kraus operators that realize the TPCP for adding back the edge $\{v_{i_k}, v_{j_k}\}$ to $G - \{v_{i_k}, v_{j_k}\}$ is

$$\left\{\frac{1}{\sqrt{m}}V_{kl}^{+}P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle + \left|v_{j_k}\right\rangle\right)\right] : l = 1, 2, \ldots, m\right\}$$
$$\bigcup\left\{\frac{1}{\sqrt{m}}V_{kl}^{-}P\left[\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle - \left|v_{j_k}\right\rangle\right)\right] : l = 1, 2, \ldots, m\right\}$$
$$\bigcup\left\{\frac{1}{\sqrt{m}}V_{il}P[|v_i\rangle] : i = 1, 2, \ldots, n;\ i \neq i_k, j_k;\ l = 1, 2, \ldots, m\right\},$$

where V_{kl}^{+}, V_{kl}^{-} and V_{il} are $n \times n$ unitary matrices defined as follows:

$$V_{kl}^{+}\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle + \left|v_{j_k}\right\rangle\right) = \frac{1}{\sqrt{2}}\left(\left|v_{i_l}\right\rangle - \left|v_{j_l}\right\rangle\right), \quad \text{for } l = 1, 2, \ldots, m;$$
$$V_{kl}^{-}\frac{1}{\sqrt{2}}\left(\left|v_{i_k}\right\rangle - \left|v_{j_k}\right\rangle\right) = \frac{1}{\sqrt{2}}\left(\left|v_{i_l}\right\rangle - \left|v_{j_l}\right\rangle\right), \quad \text{for } l = 1, 2, \ldots, m;$$
$$V_{il}|v_i\rangle = \frac{1}{\sqrt{2}}\left(\left|v_{i_l}\right\rangle - \left|v_{j_l}\right\rangle\right), \quad \text{for } i = 1, 2, \ldots, n;$$
$$i \neq i_k, j_k;\ l = 1, 2, \ldots, m.$$

5.2. Deleting and Adding a Vertex

Here we describe how to delete or add a vertex by means of TPCP. Let G be a graph on n vertices, $v_1, v_2, \ldots, v_n$, and m edges, $\left\{v_{i_1}, v_{j_1}\right\}, \left\{v_{i_2}, v_{j_2}\right\}, \ldots, \left\{v_{i_m}, v_{j_m}\right\}$, where $1 \leq i_1, j_1, i_2, j_2, \ldots, i_m, j_m \leq n$. Our purpose is to delete a vertex v_i. We first delete all the edges incident to v_i (cf. Section 5.1). In this way, we obtain a new graph, say H. We then perform the following projective measurement on $\sigma(H)$: $\mathcal{M} = \{I_n - P[|v_i\rangle], P[|v_i\rangle]\}$. Given that, possible loops in H do not appear on $\sigma(H)$, when $\mathcal{M}$ is performed on $\sigma(H)$, $I_n - P[|v_i\rangle$ clicks with probability one. The state after the measurement is $\sigma(G - v_i)$, which is the state of the desired graph. Let G be a graph on n vertices, $v_1, v_2, \ldots, v_n$, and m edges, $\left\{v_{i_1}, v_{j_1}\right\}, \left\{v_{i_2}, v_{j_2}\right\}, \ldots, \left\{v_{i_m}, v_{j_m}\right\}$, where

$1 \leq i_1, j_1, i_2, j_2, \ldots, i_m, j_m \leq n$. Our purpose is to obtain the graph $G + v_i = G \uplus \{x\}$. Consider the following density matrix $\rho = (\frac{1}{2}\sum_{i=1,2} P[|u_i\rangle]) \otimes \sigma(G)$, where $\{|u_1\rangle, |u_2\rangle\}$ forms an orthonormal basis of $\mathbb{C}^2$. We associate the vertex u_i to the state $|u_i\rangle$ for $i = 1, 2$. Consider the graph $H = (\{u_1, u_2\}, \{\{u_1, u_1\}, \{u_2, u_2\}\})$. It is easy to check (cf. Equation 4.5) that $\sigma_\circ(H) = \frac{1}{2}\sum_{i=1,2} P[|u_i\rangle]$. Also observe that $\rho = \sigma(H \otimes G)$. Thus $H \otimes G$ is a graph on $2n$ vertices labeled by $u_1v_1, u_1v_2, \ldots, u_1v_n, u_2v_1, u_2v_2, \ldots, u_2v_n$ and with $2m$ edges

$$\left\{u_1v_{i_1}, u_1v_{j_i}\right\}, \ldots, \left\{u_1v_{i_m}, u_1v_{j_m}\right\}, \left\{u_2v_{i_1}, u_2v_{j_i}\right\}, \ldots, \left\{u_2v_{i_m}, u_2v_{j_m}\right\}.$$

So, $H \otimes G = H_1 \uplus H_2$, where $H_1 = (\{u_1v_1, \ldots, u_1v_n\}, \{\{u_1v_{i_1}, u_1v_{j_i}\}, \ldots, \{u_1v_{i_m}, u_1v_{j_m}\}\})$ and $H_2 = \{\{u_2v_1, \ldots, u_2v_n\}, \{\{u_2v_{i_1}, u_2v_{j_i}\}, \ldots, \{u_2v_{i_m}, u_2v_{j_m}\}\}\}$. We first delete all the edges of $H \otimes G$ which are incident to the vertex $u_2v_1 \in V(H_2)$. Now, we perform the following projective measurement on $\sigma(G \otimes H)$:

$$\mathcal{M} = \left\{ I_{2n} - \sum_{i=2}^{n} P\left[|u_2\rangle|v_i\rangle\right], \sum_{i=2}^{n} P\left[|u_2\rangle|v_i\rangle\right] \right\}.$$

The probability that $I_{2n} - \sum_{i=2}^{n} P[|u_2\rangle|v_i\rangle]$ clicks is one and the state after the measurement is $\sigma(H_1 + u_2v_1)$, where $H_1 \cong G$.

5.3. LOCC

A *local operation and classical communication* (for short, *LOCC*) is a TPCP Λ: $\mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B) \to \mathcal{B}(\mathcal{K}_A \otimes \mathcal{K}_B)$ defined in the following way. The TPCP Λ is an LOCC if, for some $n > 0$, there exist sequences of Hilbert spaces $(\mathcal{H}_A^k)_{k=1}^{n+1}$ and $(\mathcal{H}_B^k)_{k=1}^{n+1}$ with $\mathcal{H}_A^1 = \mathcal{H}_A$, $\mathcal{H}_B^1 = \mathcal{H}_B$, $\mathcal{H}_A^{n+1} = \mathcal{K}_A$ and $\mathcal{H}_B^{n+1} = \mathcal{K}_B$, such that Λ can be written in the following form $\Lambda(\sigma) = \sum_{i_1,\ldots,i_{2n}=1}^{K_1,\ldots,K_{2n}} V_{i_1,\ldots,i_{2n}}^{AB} \sigma(V_{i_1,\ldots,i_{2n}}^{AB})^\dagger$, for all $\sigma \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$. Let $I_A^n \colon \mathcal{H}_A^n \to \mathcal{H}_A^n$ and $I_B^n \colon \mathcal{H}_B^n \to \mathcal{H}_B^n$ be identity operators. In $\Lambda(\sigma)$, $V_{i_1,\ldots,i_{2n}}^{AB} \colon \mathcal{H}_A \otimes \mathcal{H}_B \to \mathcal{K}_A \otimes \mathcal{K}_B$ is given by

$$V_{i_1,\ldots,i_{2n}}^{AB} \stackrel{def}{=} \left(I_A^{n+1} \otimes W_{2n}^{i_{2n},\ldots,i_1}\right)\left(V_{2n-1}^{i_{2n-1},\ldots,i_1} \otimes I_B^n\right)\left(I_A^n \otimes W_{2n-2}^{i_{2n-2},\ldots,i_1}\right)\cdots \left(I_A^2 \otimes W_2^{i_2,i_1}\right)\left(V_1^{i_1} \otimes I_B^1\right).$$

The sequences $\left(V_{2k-1}^{i_{2k-1},\ldots,i_1} : \mathcal{H}_A^k \longrightarrow \mathcal{H}_A^{k+1}\right)_{k=1}^n$ and $\left(W_{2k}^{i_{2k},\ldots,i_1} : \mathcal{H}_B^k \to \mathcal{H}_B^{k+1}\right)_{k=1}^n$ are families of operators. For each sequence of indices $(i_{2k}, \ldots, i_1)$ and for $k = 0, 1, \ldots, n-1$, $\sum_{i_{2k+1}=1}^{K_{2n+1}} \left(V_{2k+1}^{i_{2k+1},\ldots,i_1}\right)^\dagger V_{2k+1}^{i_{2k+1},\ldots,i_1} = I_A^{k+1}$; for each sequence of indices $(i_{2k-1}, \ldots, i_1)$ and for $k = 0, 1, \ldots, n$, $\sum_{i_{2k+2}=1}^{K_{2k+2}} \left(W_{2k+2}^{i_{2k},\ldots,i_1}\right)^\dagger W_{2k+2}^{i_{2k},\ldots,i_1} = I_B^k$.

Thermodynamic Principle. One can not obtain an entangled state from a separable state by using LOCC.

A consequence of this principle is that, given two (possibly isomorphic) graphs G and H on $n = pq$ vertices, we can always obtain $\sigma(H)$ from $\sigma(G)$ by using LOCC only, if $\sigma(G)$ is separable or entangled and $\sigma(H)$ is separable, in $\mathbb{C}^p \otimes \mathbb{C}^q$.

Example 5.3. Let $G \cong 2K_2$ and let $\{11,22\}, \{12,21\} \in E(G)$. Then

$$\sigma(G) = \frac{1}{2}P\left[\frac{1}{\sqrt{2}}[|1\rangle|1\rangle - [|2\rangle|2\rangle\right] + \frac{1}{2}P\left[\frac{1}{\sqrt{2}}[|1\rangle|2\rangle - [|2\rangle|1\rangle\right].$$

This density matrix is separable. Can we delete an edge of G by LOCC? The answer is no. If we can delete $\{12,21\}$ (or, equivalently, $\{11,22\}$) by LOCC, we obtain $\sigma(G - \{12,21\}) = P\left[\frac{1}{\sqrt{2}}[|1\rangle|1\rangle - [|2\rangle|2\rangle\right]$, which is entangled. This fact violates the thermodynamic principle.

Example 5.4. Let $G \cong K_4 - e$, for some edge e. Let f be the edge of G incident with the vertices of degree 3. Then $\sigma(G - f)$ is separable independent of the labeling. From G we can always obtain $G - f$ by LOCC.

Example 5.5. Lemma 4.4 together with Theorem 4.11 and the thermodynamic principle, shows that we can not obtain $K_{1,n-1}$ from K_n by LOCC.

6. Open Problems

Problem 6.1. The separability of $K_{1,n-1}$ and K_n do not depend on their labeling. Are these the only classes of graphs for which this happens? In general, give *separability criteria* for density matrices of graphs.

Problem 6.2. Let $\sigma(G)$ be entangled in $\mathbb{C}^p \otimes \mathbb{C}^q$. In general, whether a graph operation on G can be implemented by an LOCC depends on G and on its labeling. The following are natural questions:

(1) What are the most general conditions on G and on its labeling such that a graph H can be obtained from G by LOCCs?
(2) Does there exist a graph operation implemented by an LOCC independent of the labeling?
(3) Given a graph G, with specific properties, determine the set of all graphs which are obtainable from G by means of LOCCs.

Problem 6.3. Studying the realization of TPCP in relation to the tensor product of graphs.

Problem 6.4. We have calculated the concurrence of density matrices of graphs entangled in $\mathbb{C}^2 \otimes \mathbb{C}^2$. It turns out that for some graphs G the concurrence is equal to $\frac{1}{|E|}$. For some other graphs the concurrence is $\frac{1}{|E|} \pm \varepsilon$. Are these observations related to some property of the graphs?

Conjecture 6.5. *Let G be a graph ($|V| = pq$). If G has only one entangled edge then $\sigma(G)$ is entangled; if all the entangled edges of G are incident to the same vertex then $\sigma(G)$ is entangled.*

Let ρ_{AB} be a density matrix acting on $\mathbb{C}^p_A \otimes \mathbb{C}^q_B$, where $pq = n$. Let $S_\rho = \{\{p_i, |\psi_i\rangle : i = 1,2,\ldots,N\} : \rho_{AB} = \sum_{i=1}^n p_i |\psi_i\rangle_{AB}\langle\psi_i|$, where $|\psi_i\rangle_{AB} \in \mathbb{C}^p_A \otimes \mathbb{C}^q_B, 0 \leq p_i \leq 1$ and $\sum_{i=1}^N p_i = 1\}$. The *entanglement of formation* of ρ_{AB} is denoted and defined by $E_F(\rho_{AB}) = \inf_{\{p_i,|\psi_i\rangle : i=1,2,\ldots,N\} \in S_\rho} \sum_{i=1}^N p_i S(tr_X(|\psi_i\rangle_{AB}\langle\psi_i|))$, where $X = A$ or $X = B$.

Conjecture 6.6. *Let G be a graph ($|V| = pq$) with m edges. If $\sigma(G)$ is entangled in $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$ then $E_F(\sigma(G)) \approx \frac{1}{m}\sum_{k=1}^{m} E_F(\sigma(k))$, where $\sigma(k)$ is the pure density matrix associated to the k-th edge of G.*

Conjecture 6.7. *Let $\mathcal{G}_n^c$ be the set of all connected graphs on n vertices. Let $G \in \mathcal{G}_n^c$ ($|V| = pq$). Then $\max_{\mathcal{G}_n^c} E_F(\sigma(G)) = E_F(\sigma(K_{1,n-1}))$.*

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