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Conditions for Separability in Generalized Laplacian Matrices and Diagonally Dominant Matrices as Density Matrices

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Abstract

Recently, Laplacian matrices of graphs are studied as density matrices in quantum mechanics. We continue this study and give conditions for separability of generalized Laplacian matrices of weighted graphs with unit trace. In particular, we show that the Peres-Horodecki positive partial transpose condition is necessary and sufficient for separability in $\mathbb{C}^2 \otimes \mathbb{C}^q$. In addition, we present sufficient conditions for separability of generalized Laplacian matrices and diagonally dominant matrices.

Key words: density matrix, diagonally dominant matrix, entanglement, graph theory, Laplacian matrix, nonnegative matrix, partial transpose.

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1 Introduction

Due to novel applications of quantum mechanics in recent years such as quantum teleportation, quantum cryptography and quantum computing [1], there is much recent interest in studying entanglement in quantum systems. One important problem is to determine whether a given state operator is entangled or not. This is especially difficult for mixed state operators. In Ref. [2], normalized Laplacian matrices of graphs are considered as density matrices, and their entanglement properties are studied. The reason for studying this subclass of density matrices is that simpler and stronger conditions for entanglement can be found. In Ref. [3] a conjecture was proposed on a necessary and

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sufficient condition for separability of such density matrices and the conjecture was verified for some special classes of graphs.

The purpose of this paper is to further this study and give some generalizations of these results. In particular, we show that the Peres-Horodecki positive partial transpose condition is necessary and sufficient for Laplacian matrices of weighted graphs to be separable in $\mathbb{C}^2 \otimes \mathbb{C}^q$. Furthermore, we give sufficient conditions for generalized Laplacian matrices and diagonally dominant matrices to be separable in $\mathbb{C}^p \otimes \mathbb{C}^q$.

2 Density matrices, separability, and partial transpose

We use I and $\mathbf{0}$ to denote the identity matrix and the zero matrix respectively. We write the transpose and the complex conjugate transpose of a matrix (or vector) A as A^T and A^\dagger respectively. A state of a finite dimensional quantum mechanical system is described by a state operator or a density matrix ρ acting on \mathbb{C}^n which is Hermitian and positive semidefinite with unit trace. A state operator is called a pure state if it has rank one. Otherwise the state operator is mixed. An n by n density matrix ρ is separable in $\mathbb{C}^p \otimes \mathbb{C}^q$ with $n = pq$ if it can be written as $\sum_i c_i \rho_i \otimes \eta_i$ where ρ_i are p by p density matrices and η_i are q by q density matrices with $\sum_i c_i = 1$ and $c_i \geq 0$.¹ A density matrix that is not separable is called entangled. Entangled states are necessary to invoke behavior that can not be explained using classical physics and enable applications such as quantum teleportation [4] and quantum cryptography [5].

We denote the (i, j) -th element of a matrix A as A_{ij} . Let f be the canonical bijection between $\{1, \dots, p\} \times \{1, \dots, q\}$ and $\{1, \dots, pq\}$: $f(i, j) = (i-1)q + j$. For a pq by pq matrix A , if $f(i, j) = k$ and $f(i_2, j_2) = l$, we will sometimes write A_{kl} as $A_{(i,j)(i_2,j_2)}$.

Definition 1 *The (p, q) -partial transpose A^{T_B} of an n by n matrix A , where $n = pq$, is an n by n matrix given by:*

$$A_{(i,j)(k,l)}^{T_B} = A_{(i,l)(k,j)}$$

We will usually remove the prefix “ (p, q) ” if p and q are clear from context. In matrix form, the partial transpose is constructed as follows. If A is decomposed

¹ This definition can be extended to composite systems of multiple states, but here we only consider decomposition into the tensor product of two component states.

into p^2 blocks:

$$A = \begin{pmatrix} A^{1,1} & A^{1,2} & \dots & A^{1,p} \\ A^{2,1} & A^{2,2} & \dots & A^{2,p} \\ \vdots & \vdots & & \vdots \\ A^{p,1} & A^{p,2} & \dots & A^{p,p} \end{pmatrix} \quad (1)$$

where each $A^{i,j}$ is a q by q matrix, then A^{TB} is given by:

$$A^{TB} = \begin{pmatrix} (A^{1,1})^T & (A^{1,2})^T & \dots & (A^{1,p})^T \\ (A^{2,1})^T & (A^{2,2})^T & \dots & (A^{2,p})^T \\ \vdots & \vdots & & \vdots \\ (A^{p,1})^T & (A^{p,2})^T & \dots & (A^{p,p})^T \end{pmatrix} \quad (2)$$

It is clear that if A is Hermitian, then so is A^{TB} . Peres [6] introduced the following necessary condition for separability:

Theorem 1 *If a density matrix ρ is separable, then ρ^{TB} is positive semidefinite, i.e. ρ^{TB} is a density matrix.*

Horodecki et al. [7] showed that this condition is sufficient for separability in $\mathbb{C}^2 \otimes \mathbb{C}^2$ and $\mathbb{C}^2 \otimes \mathbb{C}^3$, but not for other tensor products. The property of a density matrix to have a positive semidefinite partial transpose is often referred to as the Peres-Horodecki condition for separability.

3 Laplacian matrices of graphs as density matrices

For a graph \mathcal{G} , the Laplacian matrix $L(\mathcal{G})$ is defined as $D - A$ where D is the diagonal matrix of vertex degrees and A is the adjacency matrix. The Laplacian matrix is symmetric positive semidefinite, has zero row sums and the zero eigenvalue is simple if and only if the graph is connected [8]. Let $|E|$ be the total number of edges in the graph. Then $\frac{1}{2|E|}L(\mathcal{G})$ has unit trace and is thus a density matrix. In Ref. [2] properties of such density matrices are obtained by studying the properties of the underlying graph. If A is the adjacency matrix of \mathcal{G} , let \mathcal{G}^{TB} be the graph with adjacency matrix A^{TB} . Graphically, \mathcal{G}^{TB} is obtained from \mathcal{G} as follows. Let the vertex $k = f(i, j)$ be located at coordinate (i, j) . Then \mathcal{G}^{TB} is obtained from \mathcal{G} by reflecting each edge vertically (or horizontally) around the midpoint of the edge. Fig. 1 shows an example for $p = 3$, $q = 4$.

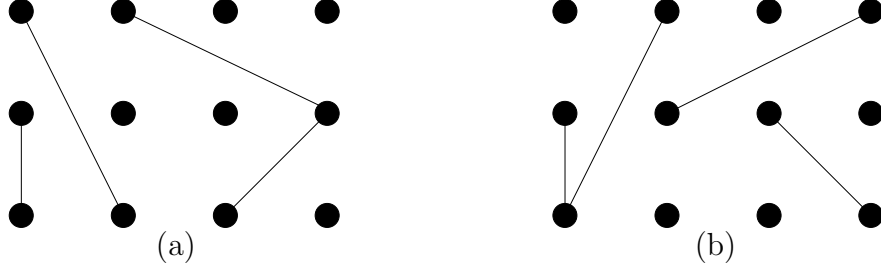


Fig. 1. (a) A graph \mathcal{G} and (b) its partial transpose \mathcal{G}^{TB} for the case $p = 3, q = 4$.

In Ref. [3] it was shown that the vertex degrees of \mathcal{G} equaling the vertex degrees of \mathcal{G}^{TB} is a necessary condition for separability and it was conjectured that this is also a sufficient condition. The sufficiency is shown for perfect matchings in $\mathbb{C}^2 \otimes \mathbb{C}^q$ and nearest point graphs.

4 Generalized Laplacian matrices of weighted graphs

Let \mathcal{S} be the set of symmetric real matrices with nonnegative row sums and nonpositive off-diagonal elements. Then \mathcal{S} is a subset of generalized Laplacian matrices as defined in Ref. [8]. We can associate a simple weighted graph to a matrix $A \in \mathcal{S}$: for $i \neq j$, $A_{ij} \neq 0$ corresponds to an edge from vertex i to vertex j with weight $-A_{ij} > 0$. Matrices in \mathcal{S} are positive semidefinite. If the corresponding graph is connected, then the smallest eigenvalue is simple. Let \mathcal{S}_1 be the matrices in \mathcal{S} with unit trace and let \mathcal{S}_1^0 be matrices in \mathcal{S}_1 with zero row sums. We focus on \mathcal{S}_1 and \mathcal{S}_1^0 which are sets of density matrices. We start with the following necessary condition for separability:

Theorem 2 *Let A be a density matrix. Let v be a vector of the form $v = w \otimes (1, \dots, 1)^T$ where w is of length p and $(1, \dots, 1)^T$ is of length q . If $Av = 0$ and $A^{TB}v \neq 0$, then A is not separable.*

Proof: Since $v_{(i,l)} = v_{(i,j)} = w_i$, this implies that

$$0 = v^\dagger Av = \sum_{ijkl} \overline{v_{(i,j)}} A_{(i,j)(k,l)} v_{(k,l)} = \sum_{ijkl} \overline{v_{(i,l)}} A_{(i,j)(k,l)} v_{(k,j)} = v^\dagger A^{TB}v$$

Next we show that v is not an eigenvector of A^{TB} . By assumption $A^{TB}v \neq 0$. If v is an eigenvector of A^{TB} , this means that v corresponds to a nonzero eigenvalue of A^{TB} which contradicts the fact that $v^\dagger A^{TB}v = 0$. Therefore $v = \sum_i a_i v_i$ is a linear combination of several eigenvectors v_i of A^{TB} , at least one of which is not in the kernel of A^{TB} with a corresponding coefficient a_i that is nonzero. Since $0 = v^\dagger A^{TB}v = \sum_i \lambda_i |a_i|^2 \|v_i\|^2$, this means that at least one of the λ_i is negative, which implies that A^{TB} is not positive semidefinite, hence by Theorem 1, A is not separable. \square

Theorem 3 *Let A be a density matrix with zero row sums. If A^{TB} does not have zero row sums, then A is not separable.*

Proof: The matrix A has zero row sums if and only if $(1, \dots, 1)^T$ is in the kernel of A . The result then follows from Theorem 2. \square

Note that Theorems 2 and 3 are applicable to general density matrices, not just Laplacian matrices of graphs. Theorem 3 generalizes Theorem 1 in Ref. [3] and is weaker than the Peres-Horodecki condition, but is easier to verify when A happens to have zero row sums. On the other hand, for matrices in \mathcal{S}_1^0 , the condition in Theorem 3 is equivalent to the Peres-Horodecki condition.

Theorem 4 *Let A be a density matrix in \mathcal{S}_1^0 . The matrix A^{TB} has zero row sums if and only if A^{TB} is positive semidefinite.*

Proof: One direction follows from the proof of Theorem 3. If A^{TB} has zero row sums, it is a matrix in \mathcal{S}_1^0 and hence positive semidefinite. \square

It is easy to show that for $A \in \mathcal{S}$ with corresponding graph \mathcal{G} , A^{TB} having the same row sums as A is equivalent to the vertex degrees of \mathcal{G} and \mathcal{G}^{TB} being equal.² For $A \in \mathcal{S}$, an edge corresponding to $A_{(i,j)(i',j')} \neq 0$ is called entangled if $i \neq i'$ and $j \neq j'$. It's easy to see that if an edge corresponding to $A_{(i,j)(i',j')}$ is not entangled, then $A_{(i,j)(i',j')} = A_{(i,j)(i',j')}^{TB}$. In Ref. [2] it was conjectured that normalized Laplacian matrices of graphs where all entangled edges are adjacent to the same vertex v are not separable. By Theorem 3 this conjecture is true. In particular, it is true for the larger set of density matrices in \mathcal{S}_1^0 since the degree of this vertex v must necessarily decrease in \mathcal{G}^{TB} .

5 Sufficient and necessary conditions for separability

Theorem 5 *Let F be a q by q matrix of the form $F = \begin{pmatrix} N \\ \mathbf{0} \end{pmatrix}$ and D be a*

q by q diagonal matrix of the form $D = \begin{pmatrix} I \\ \mathbf{0} \end{pmatrix}$ where N is a normal matrix of the same size as I . If all eigenvalues λ_i of N satisfies $|\lambda_i| \leq 1$, then the matrix

$$A = \frac{1}{2\text{Tr}(D)} \begin{pmatrix} D & F \\ F^\dagger & D \end{pmatrix}$$

² The vertex degree of v in a weighted graph is the sum of the weights of all the edges connected to v .

is a density matrix and is separable in $\mathbb{C}^2 \otimes \mathbb{C}^q$.

Proof: Since N is normal, it can be written as $N = \sum_i \lambda_i v_i v_i^\dagger$ where λ_i and v_i are the eigenvalues and eigenvectors of N respectively. Define

$$w_i = \begin{pmatrix} v_i \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

This means that $F = \sum_i \lambda_i \bar{w}_i w_i^\dagger$. Furthermore, $\sum_i v_i v_i^\dagger = I$ implies that $\sum_i w_i w_i^\dagger = D$. Define $X_i = \begin{pmatrix} 1 & \lambda_i \\ \bar{\lambda}_i & 1 \end{pmatrix} \otimes w_i w_i^\dagger$. Note that $\begin{pmatrix} 1 & \lambda_i \\ \bar{\lambda}_i & 1 \end{pmatrix}$ is positive semidefinite since $|\lambda_i| \leq 1$. Then

$$\sum_i X_i = \begin{pmatrix} \sum_i w_i w_i^\dagger & \sum_i \lambda_i w_i w_i^\dagger \\ \sum_i \bar{\lambda}_i w_i w_i^\dagger & \sum_i w_i w_i^\dagger \end{pmatrix} = \begin{pmatrix} D & F \\ F^\dagger & D \end{pmatrix}$$

which shows that A is positive semidefinite and is separable. \square

Definition 2 C is a simple circuit matrix if there exists distinct integers i_1, \dots, i_k ($k \geq 1$) such that $C_{i_m i_{m+1}} = 1$ for $m = 1, \dots, k-1$, $C_{i_k i_1} = 1$ and $C_{ij} = 0$ otherwise.

Corollary 1 If C is a q by q simple circuit matrix and D is the diagonal matrix with the row sums of C on the diagonal, then the matrix

$$A = \frac{1}{2\text{Tr}(D)} \begin{pmatrix} D & -C \\ -C^T & D \end{pmatrix}$$

is a density matrix and is separable in $\mathbb{C}^2 \otimes \mathbb{C}^q$.

Proof: By permuting the indices, we can assume that $1 \leq i_1, \dots, i_k \leq k$ in Definition 2, i.e. i_1, \dots, i_k is a permutation of $1, \dots, k$. This is equivalent to saying that there exists permutation matrices P, Q such that $Q^T C Q$ is of the form $\begin{pmatrix} P \\ \mathbf{0} \end{pmatrix}$. Therefore without loss of generality, we assume that C is of

the form $C = \begin{pmatrix} P \\ \mathbf{0} \end{pmatrix}$. This means that $D = \begin{pmatrix} I \\ \mathbf{0} \end{pmatrix}$. Since $-P$ is unitary

and thus normal with eigenvalues on the unit circle, the result follows from Theorem 5. \square

Note that A as defined in Corollary 1 is a matrix in \mathcal{S}_1^0 .

Definition 3 *A matrix is line sum symmetric if the i -th column sum is equal to the i -th row sum for each i .*

Theorem 6 *Let A be a $2q$ by $2q$ density matrix in \mathcal{S}_1 . If A^{TB} has the same row sums as A , then the matrix A is separable in $\mathbb{C}^2 \otimes \mathbb{C}^q$.*

Proof: It is easy to see that A can be decomposed into:

$$A = \begin{pmatrix} A_1 & \\ & A_2 \end{pmatrix} + \begin{pmatrix} D_1 & -B \\ -B^T & D_2 \end{pmatrix}$$

where A_1 and A_2 are symmetric matrices and D_1 and D_2 are diagonal matrices with the row sums of B and B^T on the diagonal respectively. It is easy to see that A_1 and A_2 are in \mathcal{S} and thus are positive semidefinite. The first term $\begin{pmatrix} A_1 & \\ & A_2 \end{pmatrix}$ can be separated as $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes A_1 + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes A_2$. As for the second term, B is a matrix with nonnegative entries. If A^{TB} has the same row sums as A , then B has the same row sums as B^T . This means that the i th column sum of B is equal to its i th row sum, i.e. B is line sum symmetric. Using results in network flow theory, it was shown in Ref. [9] that B can be written as $\sum_i \alpha_i C_i$, where C_i are simple circuit matrices and $\alpha_i \geq 0$. This together with Corollary 1 implies that A is separable in $\mathbb{C}^2 \otimes \mathbb{C}^q$. \square

Our main result shows that for density matrices in \mathcal{S}_1^0 , the Peres-Horodecki condition (which by Theorem 4 is equivalent to A^{TB} having zero row sums) is sufficient and necessary for separability in $\mathbb{C}^2 \otimes \mathbb{C}^q$.

Theorem 7 *Let A be a $2q$ by $2q$ density matrix in \mathcal{S}_1^0 . The matrix A is separable in $\mathbb{C}^2 \otimes \mathbb{C}^q$ if and only if A^{TB} has zero row sums.*

Proof: Follows from Theorems 3 and 6. \square

6 A sufficient condition for separability

The techniques in Section 5 can be applied to density matrices in \mathcal{S}_1 acting on the more general tensor product $\mathbb{C}^p \otimes \mathbb{C}^q$. In fact, the same arguments can be used to prove the following sufficient condition for separability:

For a normalized Laplacian matrix A of a graph such that $A_{(i,j)(i',j')} \neq 0$ implies $|i - i'| \leq 1$ and $|j - j'| \leq 1$ (the so-called nearest point graphs), it was shown in Ref. [3] via a combinatorial argument that A is separable if and only if A^{TB} has zero row sums. Corollary 3 is a generalization of this result as the condition $|j - j'| \leq 1$ is not necessary.

7 Diagonally dominant complex density matrices

Definition 4 *A matrix A is (row) diagonally dominant if $|A_{ii}| \geq \sum_{j \neq i} |A_{ij}|$ for all i .*

By Gershgorin's circle criterion [10] a diagonally dominant matrix with real nonnegative diagonal entries has eigenvalues with nonnegative real parts. Thus a Hermitian diagonally dominant matrix with nonnegative diagonal elements is positive semidefinite.

Definition 5 *For a matrix A , let $|A|$ denote the real nonnegative matrix B such that $B_{ij} = |A_{ij}|$.*

Let \mathcal{V} be the set of diagonally dominant Hermitian matrices with nonnegative diagonal elements. Let \mathcal{V}_1 be the set of matrices in \mathcal{V} with unit trace. Then each element of \mathcal{V}_1 is a density matrix. We obtain results for \mathcal{V}_1 which are analogous to those for \mathcal{S}_1 . For instance, we have the following Corollary to Theorem 5:

Corollary 4 *If C is a q by q matrix such that $|C|$ is a simple circuit matrix and D is the diagonal matrix with the row sums of $|C|$ on the diagonal, then the matrix*

$$A = \frac{1}{2\text{Tr}(D)} \begin{pmatrix} D & C \\ C^\dagger & D \end{pmatrix}$$

is a density matrix and is separable in $\mathbb{C}^2 \otimes \mathbb{C}^q$.

Proof: As in Corollary 1, without loss of generality we assume that C is of the form $C = \begin{pmatrix} X & \\ & \mathbf{0} \end{pmatrix}$ where $|X|$ is a permutation matrix. Note that X is unitary since $X^\dagger X = X X^\dagger = I$. The rest of the proof is virtually the same as that of Corollary 1. \square

Lemma 1 *For a complex number x , if $a, b \geq 0$ are real numbers such that $a + b = |x|$, then there exists x_1, x_2 such that $x_1 + x_2 = x$ and $|x_1| = a$, $|x_2| = b$.*

Proof: Pick $x_1 = \frac{ax}{|x|}$ and $x_2 = \frac{bx}{|x|}$. □

Corollary 4 and the same arguments as in Section 5 are used to prove the following:

Theorem 9 *Let A be a $2q$ by $2q$ matrix in \mathcal{V}_1 . If $|A^{TB}|$ has the same row sums as $|A|$, then the matrix A is separable in $\mathbb{C}^2 \otimes \mathbb{C}^q$.*

Proof: Recall that if $|A|$ is line sum symmetric, then $|A| = \sum_i \alpha_i C_i$ where C_i are circuit matrices. By Lemma 1 this implies that A can be written as $A = \sum_i \alpha_i A_i$ where $|A_i| = C_i$. Utilizing Corollary 4, the rest of the proof is similar to Theorem 6. □

Theorem 10 *If an n by n matrix A in \mathcal{V}_1 written in the form Eq. (1) is such that the matrices $|A^{i,j}|$ are line sum symmetric, then A is separable in $\mathbb{C}^p \otimes \mathbb{C}^q$.*

Proof: The proof is similar to Theorem 8. □

Corollary 5 *Let A be a matrix in \mathcal{V}_1 be such that $A_{(i,j)(i',j')} \neq 0$ implies that $|i - i'| \leq 1$. If $|A^{TB}|$ has the same row sums as $|A|$, then A is separable in $\mathbb{C}^p \otimes \mathbb{C}^q$.*

Proof: The proof is similar to Corollary 2. □

Theorem 11 *Consider a matrix $A \in \mathcal{V}_1$ decomposed as in Eq. (1). If for each $i \neq j$, $A^{i,j}$ is either Hermitian or skew-Hermitian, then A is separable.*

Proof: Follows from Theorem 10 and the fact if a matrix X is Hermitian or skew-Hermitian, then $|X|$ is line sum symmetric. □

Every square matrix can be decomposed as a sum of a Hermitian matrix and a skew-Hermitian matrix. This is generally written as $A = \text{Re}(A) + i\text{Im}(A)$ where $\text{Re}(A) = \frac{1}{2}(A + A^\dagger)$ and $\text{Im}(A) = -\frac{1}{2}i(A - A^\dagger)$ are Hermitian matrices. Thus a matrix A in the form Eq. (1) can be decomposed as $A = B + C$ where

$$B = \begin{pmatrix} B^{1,1} & \text{Re}(A^{1,2}) & \dots & \text{Re}(A^{1,p}) \\ \text{Re}(A^{2,1}) & B^{2,2} & \dots & \text{Re}(A^{2,p}) \\ \vdots & \vdots & & \vdots \\ \text{Re}(A^{p,1}) & \text{Re}(A^{p,2}) & \dots & B^{p,p} \end{pmatrix}$$

$$C = \begin{pmatrix} C^{1,1} & i\text{Im}(A^{1,2}) & \dots & i\text{Im}(A^{1,p}) \\ i\text{Im}(A^{2,1}) & C^{2,2} & \dots & i\text{Im}(A^{2,p}) \\ \vdots & \vdots & & \vdots \\ i\text{Im}(A^{p,1}) & i\text{Im}(A^{p,2}) & \dots & C^{p,p} \end{pmatrix}$$

with $A^{i,i} = B^{i,i} + C^{i,i}$.

Theorem 12 *If $B^{i,i}$ and $C^{i,i}$ are chosen such that B and C are in \mathcal{V}_1 , then A is separable.*

Proof: Follows from Theorem 11. □

A consequence of Theorem 12 is that a density matrix A is separable if $\min_i A_{ii}$ is much larger than $\max_i \sum_{j \neq i} |A_{ij}|$. This gives yet another proof of the fact that $\frac{1}{\text{Tr}(I+X)}(I+X)$ is separable into two component states if X is small enough [11].

The conditions in this section can sometimes be applied to density matrices which are not diagonally dominant. For instance, if

$$A = \begin{pmatrix} B^1 & & \\ & \ddots & \\ & & B^p \end{pmatrix} + C$$

where B^i are positive semidefinite and C is diagonally dominant, then A is separable if C is separable.

8 Conclusions

We study separability criteria for density matrices that can be expressed as generalized Laplacian matrices of weighted graphs or diagonally dominant matrices. In particular, we show that the well-known Peres-Horodecki necessary condition for separability is in fact sufficient for Laplacian matrices in $\mathbb{C}^2 \otimes \mathbb{C}^q$.

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