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Note

Graphs whose normalized Laplacian matrices are separable as density matrices in quantum mechanics

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ABSTRACT

Recently normalized Laplacian matrices of graphs are studied as density matrices in quantum mechanics. Separability and entanglement of density matrices are important properties as they determine the nonclassical behavior in quantum systems. In this note we look at the graphs whose normalized Laplacian matrices are separable or entangled. In particular, we show that the number of such graphs is related to the number of 0–1 matrices that are line sum symmetric and to the number of graphs with at least one vertex of degree 1.

1. Introduction

Applications of quantum mechanics in information technology such as quantum teleportation, quantum cryptography and quantum computing [5] lead to 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 Refs. [2,1,8,7,9,10], 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 and separability can be found and graph theory may shed light on the entanglement properties of state operators. In this note, we continue this study and determine the number of graphs that result in separable or entangled density matrices.

2. Density matrices, separability, and partial transpose

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 cannot be explained using classical physics and enable novel applications.

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

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[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.

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

$$A^{PT}_{(i,j)(k,l)} = A_{(i,l)(k,j)}.$$

We remove the prefix "(p, q)" if p and q are clear from context. In matrix form, the partial transpose is constructed by decomposing A into p^2 blocks

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

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

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

2.1. Necessary conditions for separability of density matrices

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

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

Horodecki et al. [4] 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. A density matrix having a positive semidefinite partial transpose is often referred to as the Peres–Horodecki condition for separability.

In [8] it was shown that when restricted to zero row sum density matrices, we have a weaker form of the Peres–Horodecki condition that is easier to verify.

Theorem 2. *If a density matrix A with zero row sums is separable, then A^{PT} has zero row sums.*

3. Normalized Laplacian matrices as density matrices

For a Laplacian matrix A of a nonempty graph, $\frac{1}{Tr(A)}A$ is symmetric positive semidefinite with trace 1 and thus can be viewed as a density matrix of a quantum system. In [1] it was shown that a necessary condition for separability of a Laplacian matrix is that the vertex degrees of the graph and its partial transpose are the same for each vertex. This condition is equivalent to row sums of A^{PT} being 0. In [8] it was shown that this condition is also sufficient for separability in $\mathbb{C}^2 \otimes \mathbb{C}^q$. Note that separability of the normalized Laplacian matrix is not invariant under graph isomorphism. Therefore the vertex numbering is important in determining separability; i.e. we consider labeled graphs. For labeled graphs of n vertices, there are $2^{\frac{n(n-1)}{2}}$ different Laplacian matrices to consider. Since the empty graph has trace 0 and cannot be considered a density matrix, we only need to look at $L(n) = 2^{\frac{n(n-1)}{2}} - 1$ different matrices.

4. A sufficient condition for separability of normalized Laplacian matrices

Definition 2. A square matrix is *line sum symmetric* if the ith column sum is equal to the ith row sum for each i.

Theorem 3 ([8])**.** *A normalized Laplacian matrix A is separable in $\mathbb{C}^p \otimes \mathbb{C}^q$ if $A^{i,j}$ in Eq. (1) is line sum symmetric for all i, j.*

For V_1 and V_2 disjoint subsets of vertices of a graph, let $e(V_1, V_2)$ denote the number of edges between V_1 and V_2. A graphical interpretation of Theorem 3 is that by splitting the pq vertices into p groups V_i of q vertices, where $V_i = \{(i-1)q+1, (i-1)q+2, \ldots, iq\}$, the normalized Laplacian matrix of a graph $\mathcal{G}$ is separable in $\mathbb{C}^p \otimes \mathbb{C}^q$ if for each $j \neq i$ and for each $1 \leq m \leq q$, $e(v, V_j) = e(w, V_i)$ where v is the mth vertex in V_i and w is the mth vertex in V_j. This is illustrated in Fig. 1 for the case $p = 2$.

Definition 3. Let $L_s(p, q)$ be the number of normalized Laplacian matrices of graphs of n vertices that are separable under $\mathbb{C}^p \otimes \mathbb{C}^q$ where $n = pq$. Let $L_e(p, q)$ be the number of normalized Laplacian matrices of graphs of n vertices that are entangled under $\mathbb{C}^p \otimes \mathbb{C}^q$.

It is clear that $L_s(p, q) + L_e(p, q) = L(pq)$.