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 [1] 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. [2–7], 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.

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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 can not 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 $A_{(i,j)(i_2,j_2)}$.

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

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

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

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

2.1 Necessary conditions for separability of density matrices

It is clear that if A is Hermitian, then so is A^{PT}. Peres [8] 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.*

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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.

Horodecki et al. [9] 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 [4] 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 [3] 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 [4] 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 sufficent condition for separability of normalized Laplacian matrices

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

Theorem 3 ([4]) *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 $V_i = \{(i-1)q+1, (i-1)q+2, ..., iq\}$, 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 m-th vertex in V_i and w is the m-th vertex in V_j. This is illustrated in Fig. 1 for the case $p = 2$.
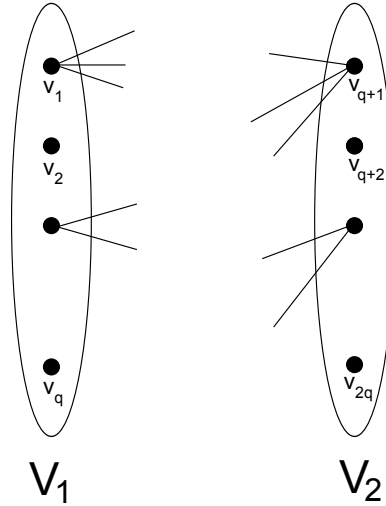
Figure 1: A sufficient condition for separability for the case $p = 2$ is that the number of edges from vertex v_i to V_2 is the same as the edges from vertex v_{q+i} to V_1 for each i.

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 $L_s(p,q) + L_e(p,q) = L(pq)$.

4.1 Upper and lower bounds for L_s and L_e

Definition 4 *Let $\mathcal{N}_s(n)$ denote the set of n by n 0-1 matrices that are line sum symmetric. Let $N_s(n)$ denote the cardinality of the set $\mathcal{N}_s(n)$. Let $\mathcal{N}_e(n)$ denote the set of n by n 0-1 matrices that are not line sum symmetric. Let $N_e(n)$ denote the cardinality of the set $\mathcal{N}_e(n)$.*

Clearly $N_s(n) + N_e(n) = 2^{n^2}$. The first few values of $N_s(n)$ can be found in `https://oeis.org/A229865`.

We now show how bounds for L_s (and L_e) can be derived from N_s.

Theorem 4
$$L_s(p,q) \geq 2^{\frac{pq(q-1)}{2}} N_s(q)^{\frac{p(p-1)}{2}} - 1$$

Proof: Let A be the normalized Laplacian matrix of a graph. Since A is symmetric, in the decomposition in Eq. (1), $A^{i,i}$ is symmetric and $A^{i,j} = (A^{j,i})^T$. Therefore to apply Theorem 3 we only need to check that $A^{i,j}$ is line sum symmetric for $j > i$. There are $\frac{p(p-1)}{2}$ such submatrices and thus $N_s(q)^{\frac{p(p-1)}{2}}$ possible combinations. The remaining entries in the strictly upper triangular portion

of A corresponds to $\frac{pq(pq-1)}{2} - \frac{p(p-1)}{2}q^2 = \frac{pq(q-1)}{2}$ elements which corresponds to $2^{\frac{pq(q-1)}{2}}$ combinations. This combines to $2^{\frac{pq(q-1)}{2}} N_s(q)^{\frac{p(p-1)}{2}}$ combinations. Finally we need to subtract 1 for the zero matrix corresponding to the empty graph. $\square$

Definition 5 *Let $\mathcal{M}_n(i)$ denote the set of symmetric n by n $0-1$ matrices such that*

- *There is at least one row with a single 1.*

- *The diagonal entries are 0*

- *There are $2i$ nonzero elements in the matrix.*

Let $M_n(i)$ denote the cardinality of the set $\mathcal{M}_n(i)$.

Some values of $M_n(i)$ are shown in Table 1. It is clear that $\mathcal{M}_n(i)$ is the set of adjacency matrices of labeled graphs of n vertices and i edges with at least one vertex of degree 1 and $M_n(i)$ is the number of such graphs.

Theorem 5 $M_n(i) = 0$ if $i > \frac{(n-1)(n-2)}{2} + 1$. For $j \geq 0$, $n \geq 4 + j$,

$$M_n\left(\frac{(n-1)(n-2)}{2} - j + 1\right) = n(n-1)\left(\begin{array}{c} \frac{(n-1)(n-2)}{2} \\ j \end{array}\right).$$

For $i \leq 3$, $M_n(i)$ is equal to the number of labeled bipartite graphs with n vertices and i edges.[2] In particular, $M_n(1) = \frac{n(n-1)}{2}$, $M_n(2) = \frac{(n+1)n(n-1)(n-2)}{8}$, $M_n(3) = \frac{((n+1)(n+2)+2)n(n-1)(n-2)(n-3)}{48}$.

Proof: Clearly the maximum number of edges in a graph with at least one vertex of degree 1 is achieved with a single vertex v connected to a vertex w in a clique of $(n-1)$ vertices, and this graph has $\frac{(n-1)(n-2)}{2} + 1$ edges. If $n \geq 4 + j$ and a graph $\mathcal{G}$ with $\frac{(n-1)(n-2)}{2} - j + 1$ edges has at least one vertex of degree 1, then this graph will have a single vertex v connected to a vertex w in a graph $\mathcal{W}$ consisting of $n-1$ vertices and $\frac{(n-1)(n-2)}{2} - j$ edges, i.e. $\mathcal{W}$ is a clique of $n-1$ vertices minus j edges. Each vertex of $\mathcal{W}$ has degree $\geq n-2-j \geq 2$, i.e. $\mathcal{W}$ does not include a vertex of degree 1. In this case $\mathcal{G}$ is uniquely defined by the vertices v and w and the graph $\mathcal{W}$. There are $n(n-1)$ such pairs of vertices (v, w) and there are $\left(\begin{array}{c} \frac{(n-1)(n-2)}{2} \\ j \end{array}\right)$ labeled graphs with $n-1$ vertices and $\frac{(n-1)(n-2)}{2} - j$ edges.

Let $\mathcal{G}$ be a graph of n vertices with at least one vertex of degree 1 and at most 3 edges. Since there are no cliques of 3 vertices, it is a bipartite graph. Similarly if $\mathcal{G}$ is a bipartite graph of at most 3 edges, the absence of cliques of 3 vertices means that there is a vertex of degree 1. $\square$

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[2]See https://oeis.org/A000217, https://oeis.org/A050534, https://oeis.org/A053526.

n	$M_n(1)$	$M_n(2)$	$M_n(3)$	$M_n(4)$	$M_n(5)$	$M_n(6)$	$M_n(7)$	$M_n(8)$
2	1							
3	3	3						
4	6	15	16	12				
5	10	45	110	195	210	120	20	
6	15	105	435	1320	2841	4410	4845	3360
7	21	210	1295	5880	19887	51954	106785	171360
8	28	378	3220	20265	97188	369950	1147000	2931138

Table 1: Values of $M_n(i)$.

Theorem 6

$$L_e(p,q) \geq \sum_{i=1}^{\frac{(p-1)(p-2)}{2}+1} M_p(i) N_e(q)^i N_s(q)^{\frac{p(p-1)}{2}-i} 2^{\frac{pq(q-1)}{2}}$$

Proof: Consider the mapping where we replace each submatrix $A^{i,j}$ with 1 if it is an element of $\mathcal{N}_e(q)$ and 0 otherwise. This results in a p by p $0-1$ matrix B. If B is in $\mathcal{M}_p(k)$ for some k, then A has a row of submatrices $A^{i,j}$ that are all line sum symmetric except for one, and this implies that A^{PT} does not have zero sums and thus A is not separable by Theorem 2. There are $M_p(k) N_e(q)^k N_s(q)^{\frac{p(p-1)}{2}-k}$ such combinations. As before, there are $\frac{pq(q-1)}{2}$ remaining locations in the strictly upper triangular part of A that is not occupied by $A^{i,j}$ for some $i \neq j$. $\qquad\square$

Corollary 1

$$L_s(p,q) \leq L(pq) - \sum_{i=1}^{\frac{(p-1)(p-2)}{2}+1} M_p(i) N_e(q)^i N_s(q)^{\frac{p(p-1)}{2}-i} 2^{\frac{pq(q-1)}{2}}$$

$$L_e(p,q) \leq L(pq) - 2^{\frac{pq(q-1)}{2}} N_s(q)^{\frac{p(p-1)}{2}} + 1$$

It is easy to show that the upper and lower bound for the case $p = 2$ coincide and this corresponds to the fact that the separability (and entanglement) condition is both sufficient and necessary in $\mathbb{C}^2 \otimes \mathbb{C}^q$ [4]. In particular,

Theorem 7

$$L_s(2,q) = 2^{q(q-1)} N_s(q) - 1$$
$$L_e(2,q) = 2^{q(q-1)} N_e(q)$$

Proof: The upper bound for $L_s(2,q)$ is equal to

$$L(2q) - N_e(q) 2^{q(q-1)} = 2^{q(2q-1)} - 1 - (2^{q^2} - N_s(q)) 2^{q(q-1)} = N_s(q) 2^{q(q-1)} - 1$$

which is also the lower bound for $L_s(2,q)$. $\qquad\square$

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