Discrete Mathematics 310 (2010) 2811–2814

Contents lists available at ScienceDirect

Discrete Mathematics

journal homepage: www.elsevier.com/locate/disc

On graphs whose Laplacian matrix's multipartite separability is invariant under graph isomorphism

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ARTICLE INFO

Article history:
Received 2 November 2009
Accepted 9 June 2010
Available online 14 July 2010

Keywords:
Laplacian matrix
Quantum mechanics
Entanglement
Density matrix
Graph isomorphism

ABSTRACT

Normalized Laplacian matrices of graphs have recently been studied in the context of quantum mechanics as density matrices of quantum systems. Of particular interest is the relationship between quantum physical properties of the density matrix and the graph theoretical properties of the underlying graph. One important aspect of density matrices is their entanglement properties, which are responsible for many nonintuitive physical phenomena. The entanglement property of normalized Laplacian matrices is in general not invariant under graph isomorphism. In recent papers, graphs were identified whose entanglement and separability properties are invariant under isomorphism. The purpose of this note is to completely characterize the set of graphs whose separability is invariant under graph isomorphism. In particular, we show that this set consists of $K_{2,2}$ and its complement, all complete graphs and no other graphs.

1. Introduction

The objects of study in this paper are density matrices of quantum mechanics. Density matrices are used to describe the state of a quantum system and are fundamental mathematical constructs in quantum mechanics. They play a key role in the design and analysis of quantum computing and information systems [4].

Definition 1. A complex matrix A is a *density matrix* if it is Hermitian, positive semidefinite and has unit trace.

Definition 2. A complex matrix A is row diagonally dominant if $A_{ii} \geq \sum_{j \neq i} |A_{ij}|$ for all i.

By Gershgorin's circle criterion, all the eigenvalues of a row diagonally dominant matrix have nonnegative real parts. Thus a nonzero Hermitian row diagonally dominant matrix is positive semidefinite and has a strictly positive trace, and such a matrix, normalized[1], is a density matrix.

A key property of a density matrix is its separability. The property of nonseparability is crucial in generating the myriad counterintuitive phenomena in quantum mechanics and is indispensable in the construction of quantum information processing systems.

Definition 3. A density matrix A is *separable* in $\mathbb{C}^{p_1} \times \mathbb{C}^{p_2} \times \cdots \times \mathbb{C}^{p_m}$ ($p_i \geq 2$) if it can be written as $A = \sum_i c_i A_i^1 \otimes \cdots \otimes A_i^m$ where $c_i \geq 0$, $\sum_i c_1 = 1$ and A_i^j are density matrices in $\mathbb{C}^{p_j \times p_j}$. A density matrix is *entangled* if it is not separable.

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[1] We define the normalization of a matrix A with nonzero trace as $\frac{1}{\mathrm{tr}(A)} A$.

0012-365X/$ – see front matter
doi:10.1016/j.disc.2010.06.014

2. Laplacian matrices as density matrices

The Laplacian matrix of a graph is defined as $L = D - A$, where D is the diagonal matrix of the vertex degrees and A is the adjacency matrix. The matrix L is symmetric and row diagonally dominant, and therefore for a nonempty[2] graph the matrix $\frac{1}{\mathrm{tr}(L)}L$ is a density matrix. In Ref. [3], such normalized Laplacian matrices are studied as density matrices and quantum mechanical properties such as entanglement of graph Laplacian matrices of various types are studied. This approach was further investigated in [6] where it was shown that the Peres–Horodecki necessary condition for separability is equivalent to a condition on the partial transpose graph, and that this condition is also sufficient for separability of block tridiagonal Laplacian matrices and Laplacian matrices in $\mathbb{C}^2 \times \mathbb{C}^q$. In Ref. [2] several classes of graphs were identified whose separabilities are easily determined. In Ref. [5] the tripartite separability of normalized Laplacian matrices is studied. Clearly separability and entanglement are only nontrivial if the order of the density matrix is composite. Therefore in this note we only consider nonempty graphs on n vertices where n is a composite integer.

As noted in Ref. [3], the separability of a normalized Laplacian matrix of a graph is not invariant under graph isomorphism; it depends on the labeling of the vertices. In the sequel, unless otherwise noted, we will assume a specific Laplacian matrix (and thus a specific vertex labeling) when we discuss separability of Laplacian matrices of graphs. To determine separability of normalized Laplacian matrices, it is more convenient for a graph of $n = p_1p_2 \cdots p_m$ vertices to consider the vertices as m-tuples in $V_1 \times V_2 \times \cdots \times V_m$, $|V_i| = p_i$.

In particular, we define a vertex labeling as follows:

Definition 4. For $n = p_1p_2 \cdots p_m$, a *vertex labeling* is a bijection between $\{1, \ldots, n\}$ and $\{1, \ldots, p_1\} \times \{1, \ldots, p_2\} \times \cdots \times \{1, \ldots, p_m\}$.

Definition 5. Given a graph $\mathcal{G}$ with vertices $V \times W$, the partial transpose graph $\mathcal{G}^{pT}$ is a graph with vertices $V \times W$ and edges defined as follows:

$\{(u, v), (w, y)\}$ is an edge of $\mathcal{G}$ if and only if $\{(u, y), (w, v)\}$ is an edge of $\mathcal{G}^{pT}$.

Note that the partial transpose graph depends on the specific labeling of the vertices. The partial transpose graph is useful in determining separability of the Laplacian matrix of a graph with the same vertex labeling. In [2,6] the following necessary condition for separability is shown:

Theorem 1. *If the normalized Laplacian matrix of $\mathcal{G}$ is separable then each vertex of $\mathcal{G}$ has the same degree as the same vertex of $\mathcal{G}^{pT}$.*

In Ref. [7] several classes of graphs were identified where the normalized Laplacian matrices' separability or entanglement is invariant under graph isomorphism. In particular, it was shown that for all noncomplete graphs of $2m$ vertices with $m \geq 3$, there is a vertex labeling that renders the normalized Laplacian matrix entangled. Computer experiments performed in Ref. [7] indicate that this is true for all noncomplete graphs with $4 < n \leq 9$ vertices where n is composite. The purpose of this note is to show that this is indeed the case for all composite $n > 4$ and this allows us to characterize completely the set of graphs whose separability is invariant under graph isomorphism.

3. Graphs whose normalized Laplacian matrix is multipartite separable for all vertex labelings

We will use the following generalization of the Pigeonhole Principle:

Theorem 2 (*Generalized Pigeonhole Principle*)**.** *If $rn + s$ or more objects are placed in n boxes, then for each $0 \leq m \leq n$ there exist m boxes with a total of at least $rm + \min(s, m)$ objects.*

Proof. We prove this by induction on m. The case $m = 0$ is trivial. Next consider the case $m = 1$. This case is well known, but we include the proof here for completeness. For $s \leq 0$, if all boxes have $r - 1 + s$ or less objects each, then there is a total of at most $(r - 1 + s)n < rn + s$ objects, a contradiction. For $s \geq 1$, if all boxes have r or less objects then there is a total of at most rn objects which is strictly less than $rn + s$, a contradiction. The case for $m = s = 1$ is also known as the Extended Pigeonhole Principle [1].

Assume the theorem is true for $m = k$ for some $0 \leq k < n$. Then there exist k boxes with a total of $rk + u$ objects where $u \geq \min(s, k)$. The number of objects in the remaining $n - k$ boxes is at least $rn + s - rk - u = r(n - k) + (s - u)$. By the $m = 1$ case, there exists a box in the remaining boxes with at least $r + \min(s - u, 1)$ objects. This means that we have $k + 1$ boxes with a total of at least $rk + u + r + \min(s - u, 1)$ objects. Since $u + 1 \geq \min(k + 1, s + 1)$, we deduce that $rk + u + r + \min(s - u, 1) = rk + r + \min(s, u + 1) \geq r(k + 1) + \min(s, k + 1, s + 1) = r(k + 1) + \min(s, k + 1)$. Thus we show that the theorem is true for $k + 1$ and the proof is complete. □

[2] A graph is *empty* if it has no edges. In this case the Laplacian matrix is the zero matrix and has zero trace.