Math. Struct. in Comp. Science (2008), *vol.* 18, *pp.* 205–219.
doi:10.1017/S0960129508006634 Printed in the United Kingdom

Combinatorial laplacians and positivity under partial transpose

ROLAND HILDEBRAND[†], STEFANO MANCINI[‡]
and SIMONE SEVERINI[§¶]

[†]*LJK Université Joseph Fourier, Tour IRMA, 51 rue des Mathématiques, 38400 St. Martin d'Hères, France*
[‡]*Dipartimento di Fisica, Università di Camerino, Via Madonna delle Carceri 9, 62032 Camerino, Italy*
[§]*Department of Computer Science, University of York, Heslington, Y010 5DD York, United Kingdom*
[¶]*Current address: Institute for Quantum Computing, University of Waterloo, 200 University Avenue, N2L 3G1 Waterloo, Canada*

Received July 2006

In Memory of Sauro Tulipani

The density matrices of graphs are combinatorial laplacians normalised to have trace one (Braunstein *et al.* 2006b). If the vertices of a graph are arranged as an array, its density matrix carries a block structure with respect to which properties such as separability can be considered. We prove that the so-called degree-criterion, which was conjectured to be necessary and sufficient for the separability of density matrices of graphs, is equivalent to the PPT-criterion. As such, it is not sufficient for testing the separability of density matrices of graphs (we provide an explicit example). Nonetheless, we prove the sufficiency when one of the array dimensions has length two (see Wu (2006) for an alternative proof).
Finally, we derive a rational upper bound on the concurrence of density matrices of graphs and show that this bound is exact for graphs on four vertices.

1. Introduction

Density matrices of graphs were introduced in Braunstein *et al.* (2006a) and Braunstein *et al.* (2006b) and are simply combinatorial laplacians normalised to have unit trace (the normalisation consists of dividing the non-zero entries by twice the cardinality of the edge set). In this way, we can associate with any graph G (with labelled vertices) a specific mixed quantum state (identified with its matrix representation), which is then called the *density matrix of* G. If the vertices of a graph are arranged in a multi-dimensional array, the density matrix of the graph carries a block structure, which can be associated with a split of the quantum system into subsystems. Each array dimension will then correspond to one subsystem, and the length of the array dimension will equal the number of pure states the subsystem can assume. It is useful to note that the combinatorial properties of the graph G up to isomorphism do not always characterise its density matrix, and therefore do not specify the physical properties of the state. This explains why we need to consider labelled graphs. In other words, we assume that graphs with different adjacency matrices (even if belonging to the same isomorphism class) have different density matrices, and hence correspond to different quantum states, whose properties can be radically different.

Studying density matrices of graphs with the tool-box provided by quantum mechanics has a twofold role: from the perspective of combinatorics, this interface can be fruitful in uncovering and re-defining graph theoretic properties; from the perspective of quantum mechanics, density matrices of graphs can be seen as 'simple' and 'highly symmetric' states. Observed in this light, the density matrices of graphs provide a restricted testing ground for a better understanding of the techniques and concepts employed in more general settings. Such an approach has particular value when considering the particular kind of developments in quantum physics and its applications that we are experiencing today.

Indeed, the study of finite-dimensional states is important in quantum information processing. This is the multidisciplinary area whose goal is to understand and exploit the information encoded in quantum states (see Nielsen and Chuang (2000) for a monograph on the subject and Alber *et al.* (2001) for a collection of overviews). The basis of this field is the interpretation of certain quantum physical entities as information carriers and their evolution in time as information processing dynamics. Such a view is giving rise to a number of discoveries and successful real-world applications, the most popularised examples being quantum communication and quantum computing. The main ingredient that is most likely to be responsible for the 'quantumness' is the concept of *entanglement*, which is a property associated with certain quantum states.

While entanglement was considered a mystery in the early stages of quantum physics, it is nowadays recognised as a precious resource, which is difficult both to create and then to preserve. Defining entanglement is not an easy task (see Bruß (2002) for an eloquent compilation of definitions). It only makes sense to talk of entanglement if one considers a system composed of at least two subsystems. Roughly speaking, the idea is that if the two parties (or, equivalently, subsystems) are *entangled*, then a complete description of the whole system does not imply a complete description of its parts, and *vice versa*. So, two entangled systems present some sort of *correlation* that does not appear to occur in the realm of classical mechanics, where complete information on the system implies a complete description of its individual parts.

From the mathematical point of view, the theory of entanglement is rich and diverse. It has branches in geometry, knots, Lie groups, positive maps, combinatorics, convex optimisation, and so on. The main problems are:

(i) determine whether a given quantum state is entangled;

(ii) determine how much entanglement is in a given quantum state;

(iii) determine the 'quality' of entanglement (for example, the problem of distillability).

As we mentioned above, density matrices of graphs are a restricted set in which these tasks can be given a special treatment. Specifically, Braunstein *et al.* (2006a), Braunstein *et al.* (2006b) and Wu (2006) considered the *Quantum Separability Problem* (QSP) for these matrices. The QSP is the computational problem of deciding whether a given quantum state is entangled or not, that is, whether it is *separable* (see Ioannou (2006) for a recent review). The QSP is equivalent to an instance of a combinatorial optimisation problem called the Weak Membership Problem and defined in Grötschel *et al.* (1988). In its complete generality the QSP is NP-hard (Gurvits 2003).

There is some evidence that the QSP for density matrices of graphs might be easier than for general density matrices. A simple necessary condition for separability is that the degrees of the vertices of G are the same as the degrees of the vertices of another graph, G', obtained from G by means of a simple operation acting on the edges. The operation is a combinatorial analogue of the linear algebraic partial transposition. In fact, here the graph G' will be called the *partially transposed graph*, and the condition for separability will be called the *degree-criterion*. Since the partial transposition is centrally involved in the famous *Peres–Horodecki criterion* for the separability of general states (Peres 1996; Horodecki *et al.* 1996) (which is also called the *Positivity under Partial Transpose Criterion*, or, for short, the *PPT-criterion*), it is natural to investigate the relationship between the degree-criterion and the PPT-criterion when they are applied to density matrices of graphs.

In this paper, we give an elementary proof that the two criteria are equivalent for density matrices of graphs. We also exhibit a simple example showing that the degree-criterion is not sufficient for testing separability of density matrices of disconnected graphs (that is, graphs with more than one connected component). Additionally, we verify the sufficiency of the degree-criterion when the dimension of one of the parties is two, thereby giving an alternative proof of a result in Wu (2006). There are four sections in the paper. After providing the necessary notions and terminology, the above observations are set out in Section 2. Section 3 is devoted to point (ii) above. In particular, we focus on the concurrence, which is a quantity associated with every density matrix and is strictly larger than zero for entangled states (Hill and Wootters 1997). We derive a simple upper bound on the concurrence of density matrices of graphs, and show the exactness of this bound for graphs with four vertices. Finally, we draw some conclusions in Section 4.

2. The degree-criterion and the PPT-criterion for density matrices of graphs

The purpose of this section is to shed further light on the QSP of the density matrices of graphs. First we give a formal statement of the QSP and define the PPT-criterion. We will then recall the notion of a combinatorial laplacian. We will go on to define the degree-criterion and prove its equivalence to the PPT-criterion. We conclude the section by showing that the degree-criterion is necessary and sufficient for testing separability of density matrices of graphs in $\mathbb{C}_A^2 \otimes \mathbb{C}_B^q$ (see also Wu (2006)). Our reference for graph theory is Godsil and Royle (2001).

2.1. *The quantum separability problem*

In the axiomatic formulation of quantum mechanics in Hilbert space, the state of a quantum mechanical system that is associated with the n-dimensional Hilbert space $\mathscr{H} \cong \mathbb{C}^n$ is identified with an $n \times n$ positive semidefinite, trace-one hermitian matrix called a *density matrix*. In Dirac notation, a unit vector in a Hilbert space $\mathscr{H} \cong \mathbb{C}^n$ is denoted by $|\psi\rangle$, where ψ is simply a label, and, given the vectors $|\varphi\rangle, |\psi\rangle \in \mathscr{H}$, the linear functional sending $|\psi\rangle$ to the inner product $\langle\varphi|\psi\rangle$ is denoted by $\langle\varphi|$. (We could easily avoid the Dirac notation here, but we use it to be consistent with the standard literature.) For any unit vector $|\psi\rangle \in \mathscr{H}$, the projector on $|\psi\rangle$ is the hermitian matrix $P[|\psi\rangle] := |\psi\rangle\langle\psi|$, which is called a *pure state*. Every density matrix can be written as a weighted sum of pure states (with real non-negative weights summing up to 1); if the sum has more than one component, the state is said to be *mixed*. According to this definition, the decomposition of a mixed density matrix into pure states is not necessarily unique. A matrix of the form $P[|\psi\rangle] \otimes P[|\varphi\rangle]$ is called a *product state*, where the symbol '$\otimes$' denotes the Kronecker or tensor product. Let S_A and S_B be two quantum mechanical systems associated with the p-dimensional and q-dimensional Hilbert spaces $\mathscr{H}_A \cong \mathbb{C}_A^p$ and $\mathscr{H}_B \cong \mathbb{C}_B^q$, respectively. The composite system S_{AB}, which consists of the subsystems S_A and S_B, is associated with the Hilbert space $\mathscr{H}_{AB} \cong \mathbb{C}_A^p \otimes \mathbb{C}_B^q$. The density matrix ρ of S_{AB} is said to be *separable* if

— $\rho = \sum_{i=1}^N p_i P[|\psi_i\rangle_A] \otimes P[|\varphi_i\rangle_B]$, where $p_i \geqslant 0$, for every $i = 1, 2, \ldots, N$, and we have $\sum_{i=1}^n p_i = 1$;

— the projectors $P[|\psi_i\rangle_A] \otimes P[|\varphi_i\rangle_B]$ are product states acting on $\mathscr{H}_{AB}$, respectively.

A density matrix ρ is said to be *entangled* if it is not separable. Entangled states cannot be prepared from separable states by means of operations acting locally on the subsystems. Although the definition given here refers to exactly two parties, entanglement can be defined equally well for systems composed of many subsystems.

2.2. *The PPT-criterion*

The PPT-criterion is based on the notion of a partial transpose. This is a common and important notion in the study of entanglement. Let ρ be a density matrix acting on the Hilbert space $\mathscr{H}_{AB} \cong \mathbb{C}_A^p \otimes \mathbb{C}_B^q$. Let

$$\{|u_1\rangle, |u_2\rangle, \ldots, |u_p\rangle\} \quad \text{and} \quad \{|w_1\rangle, |w_2\rangle, \ldots, |w_q\rangle\}$$

be orthonormal bases of $\mathbb{C}_A^p$ and $\mathbb{C}_B^q$, respectively. Let $\{|v_1\rangle, |v_2\rangle, \ldots, |v_n\rangle\}$ be an orthonormal basis of $\mathscr{H}_{AB}$, where $n = pq$. Alternatively, we can index these basis vectors with pairs (k, l). These vectors are taken as follows:

$$|v_{(k-1)q+l}\rangle = |v_{k,l}\rangle = |u_k\rangle\,|w_l\rangle, \quad k = 1, \ldots, p;\ l = 1, \ldots, q.$$

The *partial transpose* of ρ with respect to the system S_B is the $pq \times pq$ matrix, denoted by ρ^{Γ_B}, with the $\left(i, j; i', j'\right)$-th entry defined as follows:

$$[\rho^{\Gamma_B}]_{i,j;i',j'} = \langle u_i|\langle w_{j'}|\rho|w_j\rangle|u_{i'}\rangle,$$

where $1 \leqslant i, i' \leqslant p$ and $1 \leqslant j, j' \leqslant q$. The density matrix of S_{AB} can be written as

$$\rho = \begin{pmatrix} A_{11} & \ldots & A_{1p} \\ \vdots & \ddots & \vdots \\ A_{p1} & \ldots & A_{pp} \end{pmatrix}, \tag{1}$$

with $q \times q$ matrices A_{ij} acting on the space $\mathbb{C}_B^q$. The partial transpose is then realised by transposing all these matrices:

$$\rho^{\Gamma_B} = \begin{pmatrix} A_{11}^T & \dots & A_{1p}^T \\ \vdots & \ddots & \vdots \\ A_{p1}^T & \dots & A_{pp}^T \end{pmatrix}.$$

If ρ is separable, $\rho^{\Gamma_B} \geqslant 0$ (Peres 1996). However, the converse is not necessarily true, since there exist entangled states with positive partial transpose (the so-called *bound entangled states*). The failure of the PPT-criterion is then the failure of an operational characterisation of entangled states, which is computationally simple to verify. The PPT-criterion is necessary and sufficient for separability of density matrices acting on $\mathbb{C}_A^2 \otimes \mathbb{C}_B^2$ or $\mathbb{C}_A^2 \otimes \mathbb{C}_B^3$ (Horodecki *et al.* 1996); it is also necessary and sufficient for certain infinite-dimensional states (see Simon (2000), Duan *et al.* (2000), and Mancini and Severini (2007) for a brief review). It is important to mention that only one other (operational) criterion is known for detecting entanglement: the *realignment criterion* (Rudolph 2002; Chen and Wu 2003). It can detect bound entanglement, but for some states it is weaker than the PPT-criterion. Unfortunately, one can check numerically that the two criteria together do not solve the QSP for all states (Horodecki and Lewenstein 2000). Generally, the operational characterisation of entanglement is an open problem.

2.3. *Combinatorial laplacians*

In this subsection we recall the notion of a combinatorial laplacian. A *graph* $G = (V, E)$ is a pair defined as follows:

— $V(G)$ is a non-empty and finite set whose elements are called *vertices*;
— $E(G)$ 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 loops. A graph G is said to be *on n vertices* if the number of elements in $V(G)$ is n. The *adjacency matrix* of a graph on n vertices G is an $n \times n$ matrix, denoted $M(G)$, having rows and columns labelled by the vertices of G, and the ij-th 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 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 $d_G(v_i)$, is the number of edges adjacent to v_i. The *degree-sum* of G is defined and denoted

$$d_G = \sum_{i=1}^{n} d_G(v_i).$$

† We are only considering ‘simple’ graphs here.

The *degree matrix* of G is an $n \times n$ matrix, denoted $\Delta(G)$, with its ij-th entry defined by

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

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

$$L(G) := \Delta(G) - M(G).$$

According to our definition of a graph, $L(G) \neq 0$. Moreover, the laplacian of a graph G, scaled by the degree-sum of G, has trace one and is semidefinite positive. As such it has the characteristic features of a quantum mechanical density matrix, hence it would provide a link to quantum states. On the basis of this observation, we fix the following definition: the *density matrix of a graph* G is the matrix

$$\rho_G := \frac{1}{d_G} L(G).$$

Let $\mathscr{G}_n$ be the set of density matrices of graphs on n vertices. The set $\mathscr{G}_n$ is a subset of the set of all density matrices acting on the n-dimensional Hilbert space $\mathscr{H}_{AB} \cong \mathbb{C}_A^p \otimes \mathbb{C}_B^q$, where $n = pq$. The number of elements in $\mathscr{G}_n$ equals the number of graphs on n vertices, a number that grows superexponentially in n. There are many applications of laplacians. In particular, their eigensystems are a rich source of information about graphs (Mohar 1988).

It is important to note that graphs with different adjacency matrices have different density matrices, this is even the case for graphs belonging to the same isomorphism class (for example, those obtained from each other by permutation of the vertex labels). In fact, given a graph G with density matrix ρ_G, if there exists a permutation matrix P such that $P^T M(G) P = M(G')$, then $G \cong G'$. As a consequence G' has density matrix $P^T \rho_G P$.

Finally, given the density matrix ρ_G of a graph, in order to have a correspondence with a quantum state (density operator), we have to specify the basis in the Hilbert space with respect to which the quantum state (density operator) has ρ_G as matrix representation. This can be done by associating vertex labels with orthonormal vectors.

2.4. *The degree-criterion*

Let G be a graph on $n = pq$ vertices $v_1, v_2, \ldots, v_n$. These vertices are represented here as ordered pairs as follows:

$$v_{(k-1)p+l} = (u_k, w_l) \equiv u_k w_l, \quad k = 1, \ldots, p; \; l = 1, \ldots, q.$$

By respecting this labelling, we associate G with the orthonormal basis

$$\{|v_i\rangle : i = 1, 2, \ldots, n\} = \{|u_j\rangle \otimes |w_k\rangle : j = 1, 2, \ldots, p; k = 1, 2, \ldots, q\}$$

of the Hilbert space $\mathscr{H}_{AB} \cong \mathbb{C}_A^p \otimes \mathbb{C}_B^q$, where

$$\{|u_j\rangle : j = 1, 2, \ldots, p\} \quad \text{and} \quad \{|w_k\rangle : k = 1, 2, \ldots, q\}$$

are orthonormal bases of the Hilbert spaces $\mathscr{H}_A \cong \mathbb{C}^p$ and $\mathscr{H}_B \cong \mathbb{C}^q$, respectively. The *partial transpose of a graph* $G = (V, E)$ (with respect to $\mathscr{H}_B$), denoted $G^{\Gamma_B} = (V, E')$, is the graph such that

$$\{u_i w_j, u_k w_l\} \in E' \quad \text{if and only if} \quad \{u_i w_l, u_k w_j\} \in E.$$

If $\Delta(G) = \Delta\left(G^{\Gamma_B}\right)$, we say that G satisfies the *degree-criterion*. The following conjecture was proposed in Braunstein *et al.* (2006b): a density matrix ρ_G of a graph on $n = pq$ vertices is separable in $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$ if and only if $\Delta(G) = \Delta\left(G^{\Gamma_B}\right)$. A proof of this conjecture would give a simple method for testing the separability of density matrices of graphs, as we would only need to check whether the $n \times n$ diagonal matrices $\Delta(G)$ and $\Delta\left(G^{\Gamma_B}\right)$ are equal. There are counterexamples to this conjecture when the graph has isolated vertices (that is, vertices not belonging to any edge). This is the case for the graph G defined on a 3×3 array with laplacian

$$L(G) = \begin{pmatrix} I_4 & 0 & -I_4 \\ 0 & \vdots & 0 \\ -I_4 & 0 & I_4 \end{pmatrix}$$

where I_d is the d-dimensional identity matrix. Indeed, G satisfies the degree-criterion, but ρ_G is entangled. However, we do not have any counterexample for connected graphs yet.

The following are some known partial results for separability:

— Let ρ_G be the density matrix of a graph on $n = pq$ vertices. If ρ_G is separable in $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$, then $\Delta(G) = \Delta\left(G^{\Gamma_B}\right)$ (Braunstein *et al.* 2006b).

— If G is a nearest point graph on $n = pq$ vertices, then the density matrix ρ_G is separable in $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$ if and only if $\Delta(G) = \Delta\left(G^{\Gamma_B}\right)$ (Braunstein *et al.* 2006b).
(It may be worth recalling the definition of a nearest point graph. Consider a rectangular lattice with pq points arranged in p rows and q columns such that the distance between two neighbouring points on the same row or in the same column is 1. A *nearest point graph* is a graph whose vertices are identified with the points of the lattice and with edges having length 1 or $\sqrt{2}$.)

— Let G and H be two graphs on $n = pq$ vertices. If ρ_G is separable in $\mathbb{C}^p \otimes \mathbb{C}^q$ and $G \cong H$ (that is, G and H are isomorphic), then ρ_H is not necessarily separable in $\mathbb{C}^p \otimes \mathbb{C}^q$. However, there are exceptions, as observed by the following point (Braunstein *et al.* 2006a).

— Let K_n be the *complete graph* on n vertices. Recall that the complete graph is the graph with an edge between any pair of vertices. One can show that, for any $n = pq$, the density matrix ρ_{K_n} is separable in $\mathbb{C}^p \otimes \mathbb{C}^q$. Notice that for a graph H such that $M(H) = M(G) \otimes M(G')$ for some graphs G and G', the density matrix ρ_H is separable. Of course, if a density matrix ρ_G is separable, it does not necessarily mean that $M(G)$ is a tensor product. The *star graph* on n vertices $v_1, v_2, \ldots, v_n$, denoted $K_{1,n-1}$, is the graph whose set of edges is $\{\{v_1, v_i\} : i = 2, 3, .., n\}$. The density matrix $\rho_{K_{1,n-1}}$ is entangled for $n = pq \geqslant 4$. So, the separability properties of complete graphs and star graphs do not depend on the labelling. It is an open problem to determine if these graphs are the only ones with this property (Braunstein *et al.* 2006a).

— If ρ_G is the density matrix of a graph on $n = 2q$ vertices, then $\rho_G^{\Gamma_B} \geqslant 0$ if and only if ρ_G is separable in $\mathbb{C}_A^2 \otimes \mathbb{C}_B^q$. Equivalently, the PPT-criterion is necessary and sufficient to test separability in this case (Wu 2006).

— Wu (2006) considered generalised laplacians. Let S be the set of density matrices with non-negative row sums and non-positive off-diagonal entries. If a density matrix $\rho \in S$ of dimension $n = pq$ is such that the matrices A_{ij} (as in Equation 1) are line sum symmetric, then ρ is separable in $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$. A matrix is *line sum symmetric* if the i-th column sum is equal to the i-th row sum for each i.
As a corollary, Wu (2006) proved that if a density matrix $\rho \in S$ of dimension $n = pq$ and with zero row sums is such that $[\rho]_{i,j;i',j'} \neq 0$ implies that $|i - i'| \leqslant 1$, then ρ is separable in $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$ if and only if ρ^{Γ_B} has zero row sums (Corollary 3). This result generalises the separability of nearest point graphs. In fact, for a nearest point graph the condition $|j - j'| \leqslant 1$ is also required. It is relevant to point out here that ρ^{Γ_B} has zero row sum if and only if the degree-criterion if satisfied.

2.5. *Equivalence of the degree- and PPT-criteria*

Here we prove that for laplacians the PPT-criterion is equivalent to the degree-criterion.

Observation 1. Let ρ be a matrix acting on $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$ and satisfying the PPT-criterion, and $x \otimes y$ be a separable vector in $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$. Then the condition $\rho(x \otimes y) = 0$ implies the condition $\rho^{\Gamma_B}(x \otimes \overline{y}) = 0$. In fact, we have

$$(x \otimes y)^* \rho (x \otimes y) = (x \otimes \overline{y})^* \rho^{\Gamma_B} (x \otimes \overline{y}) = 0,$$

and by the positivity of ρ^{Γ_B}, it follows that $\rho^{\Gamma_B} (x \otimes \overline{y}) = 0$.

Here the star denotes adjoint and the overbar denotes complex conjugation. A simple proof of Braunstein *et al.* (2006b, Theorem 2) can be derived from this result, with x and y being equal to the all-ones vector.

Observation 2. As a consequence of Observation 1, if ρ is a separable density matrix and

$$\rho = \sum_{k=1}^{N} (x_k \otimes y_k)(x_k \otimes y_k)^*$$

is a separable decomposition of ρ, then, for any $k = 1, 2, \ldots, N$, we have the following conditions:

— $(x_k \otimes y_k) \in range(\rho)$;
— $(x_k \otimes \overline{y}_k) \in range(\rho^{\Gamma_B})$.

Theorem 1. Let ρ_G be the density matrix of a graph G. Then ρ_G satisfies the PPT-criterion if and only if it satisfies the degree-criterion.

Proof. We have $\rho_G (e \otimes e) = 0$, because ρ_G is the laplacian of G scaled by some coefficient, where e is the all-ones vector of the required dimension. Suppose that the degree-criterion is satisfied. Then $\rho_G^{\Gamma_B} = \rho_{G^{\Gamma_B}}$. Hence $\rho_G^{\Gamma_B}$ is positive. It follows that ρ_G satisfies the PPT-criterion. Suppose that the PPT-criterion is satisfied. Then, by Observation 1, we have that $\rho_G^{\Gamma_B} (e \otimes e) = 0$. This is exactly the degree-criterion on ρ_G. □

2.6. *Separability in* $\mathbb{C}_A^2 \otimes \mathbb{C}_B^q$

Here we prove that the degree-criterion is necessary and sufficient to test separability in $\mathbb{C}_A^2 \otimes \mathbb{C}_B^q$ of density matrices of graphs, therefore giving an alternative proof to a result in Wu (2006).

Theorem 2. Let G be a graph on $n = 2q$ vertices. Then ρ_G is separable in $\mathbb{C}_A^2 \otimes \mathbb{C}_B^q$ if and only if the degree-criterion is satisfied.

Proof. The implication '$\Rightarrow$' is easily verified. We prove the implication '$\Leftarrow$'. If G satisfies the degree-criterion, we can write

$$\rho_G = L_1 + L_2 + L_3,$$

where

$$L_1 := \begin{pmatrix} X_1 & 0 \\ 0 & 0 \end{pmatrix}, L_2 := \begin{pmatrix} 0 & 0 \\ 0 & X_2 \end{pmatrix} \text{ and } L_3 := \begin{pmatrix} X_3 & X_4 \\ X_4^T & X_3 \end{pmatrix}$$

and $X_1, \ldots, X_4$ are appropriate matrices. Now, L_1 and L_2 are trivially separable. The matrix L_3 is separable because it is a PSD block-Töplitz matrix. Hence, ρ_G is separable. $\square$

3. Concurrence

In this section we focus on the concurrence of the density matrices of graphs. The notion of concurrence was introduced in Hill and Wootters (1997). The concurrence of a density matrix acting on $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$ is a quantity that is strictly larger than zero if the state is entangled and zero if it is separable. It is defined as follows: if $|\psi\rangle_{AB} \in \mathbb{C}_A^p \otimes \mathbb{C}_B^q$, the *concurrence* of $|\psi\rangle_{AB}$ is denoted and defined by

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

where

$$\rho_A = \operatorname{tr}_B(|\psi\rangle_{AB}\langle\psi|).$$

Let ρ_{AB} be a density matrix acting on $\mathbb{C}_A^p \otimes \mathbb{C}_B^q$. The concurrence of ρ_{AB} is denoted and defined as

$$\mathscr{C}(\rho_{AB}) = \inf\left\{\sum_i \omega_i \mathscr{C}(\psi_i) : \rho_{AB} = \sum_i \omega_i |\psi_i\rangle_{AB}\langle\psi_i|, 0 \leqslant \omega_i \leqslant 1, \sum_i \omega_i = 1\right\}.$$

Now let $p = q = 2$ and

$$\sigma_y = -i|1\rangle\langle 2| + i|2\rangle\langle 1|,$$

where $|1\rangle$ and $|2\rangle$ are the eigenvectors of the matrix

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

corresponding to the eigenvalues 1 and -1, respectively. An analytical formula for $\mathscr{C}(\rho_{AB})$ is given by

$$\mathscr{C}(\rho_{AB}) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\},$$

where $\lambda_1, \lambda_2, \lambda_3$ and λ_4 are the square roots of the eigenvalues of $\rho_{AB}\widetilde{\rho}_{AB}$ arranged in decreasing order and

$$\widetilde{\rho}_{AB} := (\sigma_y \otimes \sigma_y)\rho_{AB}^T(\sigma_y \otimes \sigma_y).$$

The importance of the concurrence stems from its relation with the so-called *entanglement of formation*, which is the most widely accepted measure of entanglement (see Bennett *et al.* (1996); see also Plenio and Virmani (2006)). For a pure state (that is a state of the form $P\left[|\psi\rangle\right]$) of a system S_{AB}, a good measure of entanglement is the entropy of the density matrix associated with one of the two subsystems. Choosing the system S_A, this can be written as

$$E(\psi) := -\mathrm{tr}(\rho_A \log_2 \rho_A),$$

where

$$\rho_A = \mathrm{tr}_B(P\left[|\psi\rangle\right]).$$

For a mixed state ρ, the entanglement of formation is defined by

$$E_f(\rho) := \min \sum_i p_i E(\psi_i),$$

where the minimum is taken over all pure-state decompositions of the density matrix ρ. It is evident that computing E_f is, in general, not an easy task. Explicit formulas are only known for very specific classes of states, such as the Werner states (Vollbrecht and Werner 2001). The role of concurrence is explained by the following result (Wootters 1998). Let ρ be a mixed-density matrix of dimension 4. Then

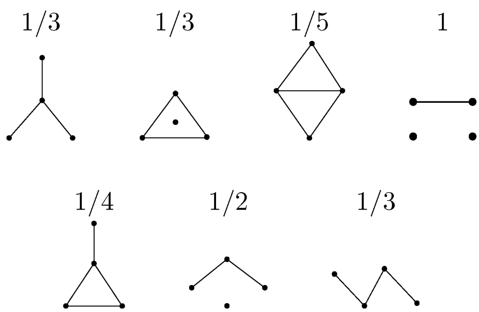
$$E_f(\rho) = H\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - \mathscr{C}(\rho)^2}\right),$$

where

$$H(x) = -x \ln x - (1 - x)\ln(1 - x)$$

is the standard information-theoretic entropy. Remarkably, $E_f(\rho)$ increases monotonically as a function of $\mathscr{C}(\rho)$.

For density matrices of graphs of dimension 4 the situation can be described as follows. There are twelve non-isomorphic graphs on 4 vertices. Seven of these graphs can have entangled density matrices. The tables below present these graphs and their respective concurrences:



Notice that in all cases the value of the concurrence is 1 over the number of edges. Moreover, one easily sees that the optimal decomposition of the density matrices of these graphs just corresponds to the decomposition of the combinatorial laplacians as sums of laplacians of 1-edge graphs.

This motivates the following definitions.

Definition 1. Let $G = (V, E)$ be a graph with its $n = pq$ vertices arranged in a $p \times q$ array. We say an edge $e \in E$ is *separable* if the density matrix of the 1-edge graph $G_e = (V, \{e\})$ is separable. We call $e \in E$ *matched* if $e \in E'$, and *unmatched* otherwise.

Recall that E' is the set of edges of the partially transposed graph G'. Thus an edge is matched if and only if it is part of a criss-cross† or it is separable. Since graphs consisting of a criss-cross give rise to separable density matrices, we have the following results.

Observation 3. Let $G = (V, E)$ be as above, and $E_1 \subset E$ be the subset of all matched edges. Then the graph $G_1 = (V, E_1)$ has a separable density matrix.

Observation 4. Let $G = (V, \{e\})$ be a 1-edge graph with its $n = pq$ vertices arranged in a $p \times q$ array, and let ρ_e be its density matrix. Then the concurrence of ρ_e is given by 0 if e is a separable edge and by 1 if e is not separable, and hence unmatched.

Corollary 2. Let $G = (V, E)$ be as above, and let n_1 be the number of matched edges of G and n_2 be the number of unmatched edges. Then the concurrence of the density matrix ρ of G is bounded from above by

$$\mathscr{C}(\rho) \leqslant \frac{n_2}{n_1 + n_2}.$$

In particular, for any graph G with density matrix ρ, we have $\mathscr{C}(\rho) \leqslant 1$.

Proof. Assume the above notation, and let ρ_1, ρ_2 be the density matrices of the graphs (V, E_1) and (V, E_2), respectively, where E_1 is the set of matched edges and E_2 the set of

† A *criss-cross* is a set $\{\{(k,i),(l,j)\},\{(k,j),(l,i)\}\}$ of two edges belonging to a set of (vertex-disjoint) entangled edges on $n = pq$ vertices (see also Braunstein *et al.* (2006a)).

unmatched edges. Then the density matrix ρ of G is given by the convex combination

$$\rho = \frac{n_1}{n_1+n_2}\rho_1 + \frac{n_2}{n_1+n_2}\rho_2\,,$$

and the density matrix ρ_2 is given by

$$\rho_2 = \frac{1}{n_2}\sum_{e\in E_2}\rho_e\,,$$

where ρ_e is the density matrix of the 1-edge graph $(V,\{e\})$. By convexity of the concurrence and by Observations 3 and 4, we obtain

$$\mathscr{C}(\rho) \leqslant \frac{n_1}{n_1+n_2}\mathscr{C}(\rho_1) + \sum_{e\in E_2}\frac{1}{n_1+n_2}\mathscr{C}(\rho_e) = \frac{n_2}{n_1+n_2}. \qquad \square$$

For all of the above graphs on four vertices, either the density matrix is separable or we have $n_2 = 1$, in which case 1 over the number of edges is an upper bound for the concurrence. As can be seen from the table, the bound is actually achieved.

The concurrences of graph density matrices that have rank 2 are listed in Hildebrand (2006). Examples IVb, IVc and IX in Hildebrand (2006) or the tally-mark† show that, in general, the upper bound is not exact, even for graphs on 2×3 arrays.

Definition 3. We say a graph $G = (V,E)$ is *maximally entangled* if the concurrence of its density matrix ρ is given by $\mathscr{C}(\rho) = 1$.

Hence, all edges of a maximally entangled graph must be unmatched.

Some questions arise naturally:

— Are there non-isomorphic graphs with the same concurrence?

— How can graphs with rational concurrence be characterised?

— Is the concurrence of ρ_G related to specific combinatorial properties of G?

— Can the set of edges of a graph $G = (V,E)$ with density matrix ρ always be partitioned into two subsets E_1, E_2 such that the density matrix of (V,E_1) is separable, (V,E_2) is maximally entangled and

$$\mathscr{C}(\rho) = \frac{\#E_2}{\#E}\,?$$

— How can maximally entangled graphs be characterised?

— Does there exist a class of density matrices of graphs for which testing separability is a difficult problem?

It might be that the existence of such a class would provide a transparent proof that detecting entanglement is hard.

† A *tally-mark* is 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 $k < l$, $s \geqslant 0$ and $i_1 < i_2 < \cdots < i_{s+2}$, belonging to a set of (vertex-disjoint) entangled edges on $n = pq$ vertices (see also Braunstein *et al.* (2006a)). Note that a criss-cross is a tally-mark with two edges.

Unfortunately, explicit formulae for computing the concurrence of density matrices are only known currently for dimensions $n \leqslant 4$ (Rungta *et al.* 2001; Li and Zhu 2003; Mintert *et al.* 2005) and for density matrices of rank 2 (Hildebrand 2006). This is an obstacle when it comes to thinking about the questions above. Nevertheless, one can still hope to find an *ad-hoc* formula for $\mathscr{C}(\rho)$, when ρ is the density matrix of a graph. In fact, it may well be that the optimal decompositions of ρ_G into pure states are very special. Finding such a formula would be interesting in view of potential generalisations.

Putting the concurrence to one side, one may ask if there is some entanglement measure specifically tailored for ρ_G. Considering the apparent success of the degree-criterion, a naive measure would be the normalised Euclidean norm $EN(\rho_G) := \|\Delta(G) - \Delta(G^{\Gamma_B})\|$. The *logarithmic negativity* is a well-known entanglement measure, and it is defined by $LN(\rho_G) := \log_2(1 + 2\mathcal{N}(\rho_G))$, where $\mathcal{N}(\rho_G)$ is the sum of the magnitudes of all negative eigenvalues of $\rho_G^{\Gamma_B}$ (Vidal and Werner 2002). There are examples of graphs G and H for which $EN(\rho_G) = EN(\rho_H)$ but $LN(\rho_G) \neq LN(\rho_H)$ (Gosh 2006).

4. Conclusion

We have proved that the degree-criterion is equivalent to the PPT-criterion. It is thus, in general, not sufficient for the separability of the density matrices of graphs. As a matter of fact, we have provided a counterexample within graphs having isolated vertices. Nevertheless, we have been able to prove the sufficiency of the degree-criterion when one of the subsystems has dimension two. In particular, as a corollary of Theorem 2, one can easily obtain the separability of criss-crosses and tally-marks.

We have also considered the concurrence as a possible entanglement measure of density matrices of graphs. There could be more suitable entanglement measures for states like this, especially as no explicit formula for concurrence is known when $n > 4$ and the rank of the density matrix is greater than 2. Further studies are required on the subject of the density matrices of graphs. However, we believe that such states provide a restricted testing ground for achieving a better understanding of the techniques and concepts employed in more general settings.

References

Alber, G. *et al.* (eds.) (2001) Quantum Information: An Introduction to Basic Theoretical Concepts and Experiments. *Springer-Verlag Tracts in Modern Physics* **173**.

Bennett, C. H., DiVincenzo, D. P., Smolin J. A. and Wootters W. K. (1996) Mixed-state entanglement and quantum error correction. *Phys. Rev. A* **54** (5) 3824–3851. (quant-ph/9604024.)

Braunstein, S. L., Ghosh, S. and Severini, S. (2007) The laplacian of a graph as a density matrix: a basic combinatorial approach to separability of mixed states. (To appear in *Ann. Comb.*) (quant-ph/0406165.)

Braunstein, S. L., Ghosh, S., Mansour, T. Severini, S. and Wilson, R. C. (2006) Some families of density matrices for which separability is easily tested. *Phys. Rev. A* **73** (1) 012320. (quant-ph/0508020.)

Bruß, D. (2002) Characterizing entanglement. Quantum information theory. *J. Math. Phys.* **43** (9) 4237–4251. (quant-ph/0110078.)

Chen, K. and Wu, L.-A. (2003) A matrix realignment method for recognizing entanglement. *Quantum Inf. and Comput.* **3** (3) 193–202. (quant-ph/0205017.)

Duan, L. M., Giedke, G., Cirac, J. I. and Zoller, P. (2000) Inseparability criterion for continuous variable systems. *Phys. Rev. Lett.* **84** 2722–2725. (quant-ph/9908056.)

Ghosh, S. (2006) Personal communication.

Godsil, C. and Royle, G. (2001) Algebraic graph theory. *Springer-Verlag Graduate Texts in Mathematics* **207**.

Grötschel, M., Lovász, L. and Schrijver, A. (1988) *Geometric Algorithms and Combinatorial Optimization*, Springer-Verlag.

Gurvits, L. (2003) Classical deterministic complexity of Edmonds' Problem and quantum entanglement. *Proceeding of the thirty-fifth ACM Symposium on Theory of Computing*, ACM Press 10–19. (quant-ph/0303055.)

Hildebrand, R. (2006) Concurrence of Lorentz-positive maps. (quant-ph/0612064.)

Hill, S. and Wootters, W. K. (1997) Entanglement of a Pair of Quantum Bits. *Phys. Rev. Lett.* **78** 5022–5025.

Horodecki, M., Horodecki, P. and Horodecki, R. (1996) Separability of mixed states: necessary and sufficient conditions. *Phys. Lett. A* **223** (1–2) 1–8. (quant-ph/9605038.)

Horodecki, P. and Lewenstein, M. (2000) Bound entanglement and continuous variables. *Phys. Rev. Lett.* **85** (13) 2657–2660. (quant-ph/0001035.)

Ioannou, L. M. (2006) Deterministic Computational Complexity of the Quantum Separability Problem. (quant-ph/0603199.)

Li, Y.-Q. and Zhu, G.-Q. (2003) Concurrence Vectors for Entanglement of High-dimensional Systems. (quant-ph/0308139.)

Mintert, F., Kuś, M. and Buchleitner, A. (2005) Concurrence of mixed multipartite quantum states. *Phys. Rev. Lett.* **95** (26) 260502. (quant-ph/0411127.)

Mohar, B. (1988) The Laplacian spectrum of graphs. In: *Graph theory, combinatorics, and applications*, Vol. 2, Kalamazoo.

Nielsen, M. and Chuang, I. (2000) *Quantum Computation and Quantum Information*, Cambridge University Press.

Peres, A. (1996) Separability criterion for density matrices, *Phys. Rev. Lett.* **77** (8) 1413–1415. (quant-ph/9604005.)

Plenio, M. B. and Virmani, S. (2005) An introduction to entanglement measures. (quant-ph/0504163.)

Rudolph, O. (2005) Further results on the cross norm criterion for separability. *Quantum Inf. Process.* **4** (3) 219–239. (quant-ph/0202121.)

Rungta, P., Bužek, V., Caves, C. M. Hillery, M. and Milburn, G. J. (2001) Universal state inversion and concurrence in arbitrary dimensions. *Phys. Rev. A* **64** (4) 042315. (quant-ph/0102040.)

Simon, R. (2000) Peres-Horodecki Separability Criterion for Continuous Variable Systems. *Phys. Rev. Lett.* **84** 2726–2729. (quant-ph/9909044.)

Mancini, S. and Severini, S. (2007) The Quantum Separability Problem for Gaussian States, In: Proceedings of Logic, Models and Computer Science 2006. *Electronic Notes in Theoretical Computer Science* **169** 121–127. (cs.CC/0603047.)

Vidal, G. and Werner, R. (2002) Computable measure of entanglement. *Phys. Rev. A* **65** 032314.

Vollbrecht, K. G. H. and Werner, R. (2001) Entanglement measures under symmetry. *Phys. Rev. A* **64** 062307. (quant-ph/0010095.)

Wu, C.-W. (2006) Conditions for separability in generalized Laplacian matrices and diagonally dominant matrices as density matrices. *Phys. Lett. A* **351** (1-2) 18–22. (quant-ph/0508163.)

Wootters, W. K. (1998) Entanglement of Formation of an Arbitrary State of Two Qubits. *Phys. Rev. Lett.* **80** 2245–2248.