Zero discord quantum states arising from weighted digraphs

Supriyo Dutta
Department of Mathematics
Indian Institute of Technology Jodhpur
Email: dutta.1@iitj.ac.in

Bibhas Adhikari
Department of Mathematics
Indian Institute of Technology Kharagpur
Email: bibhas@maths.iitkgp.ernet.in

Subhashish Banerjee
Department of Physics
Indian Institute of Technology Jodhpur
Email: subhashish@iitj.ac.in

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Abstract

In this paper we determine the class of quantum states whose density matrix representation can be derived from graph Laplacian matrices associated with a weighted directed graph and we call them graph Laplacian quantum states. Then we obtain structural properties of these graphs such that the corresponding graph Laplacian states have zero quantum discord by investigating structural properties of clustered graphs which provide a family of commuting normal matrices formed by the blocks of its Laplacian matrices. We apply these results on some important mixed quantum states, such as the Werner, Isotropic, and X-states.
1 Introduction

A strong interest has been generated towards applying graphs in different aspects of quantum mechanics and quantum information in recent times, for example, see [1, 2, 3, 4, 5, 6]. Quantum states defined by using combinatorial Laplacian and signless Laplacian matrices associated with a weighted directed graph have recently been introduced and investigated in [7]. Throughout the paper we call these quantum states as graph Laplacian states. In this paper we derive certain conditions on structure of weighted directed graphs such that the graph Laplacian quantum states have quantum discord zero. The results produced in this paper can be considered as the generalized version of the conditions for zero quantum discord of states defined by simple graphs in [8].

Recall that quantum discord \( D(\rho) \) of a state \( \rho \) is a class of quantum correlations which has been used as a resource in quantum information and communication [9, 10, 11, 12, 13, 14]. From the perspective of computational complexity, it is proved that calculating \( D(\rho) \) is an NP-complete problem [15]. This calls for developing alternate measures and techniques to realize quantum discord. A set of analytical criteria for zero and non-zero quantum discord are constructed in [16, 17]. Indeed it has been proved that a density matrix represents a quantum state with zero discord if its blocks form a family of commuting normal matrices [16]. In this paper we exploit this condition for graph Laplacian states and determine the structural properties of a graph for which this condition is met. Hence just by observing the structural properties of the graph, the zero or non zero discord quantum states can be determined.

Consider a bipartite system of order \( m \times n \). Then the density matrix corresponding to such a bipartite system is of order \( mn \times mn \) and it is a block matrix having each block of size \( n \). Treating a graph as a clustered graph on \( mn \) vertices in which each cluster contains \( n \) vertices, the combinatorial Laplacian matrix and the signless Laplacian matrix (defined in Section 2) define block density matrices corresponding to the graph. Now note that the commuting normality property of blocks of the graph Laplacian states are determined by the structural properties of the clusters of the graph. Thus if the clusters of a weighted digraph satisfy those structural properties, the corresponding graph Laplacian states have zero quantum discord. As a biproduct of this observation, it would be an easier task to construct zero quantum discord states by using the formulation developed in this paper. This approach can be considered as a combinatorial approach to construct zero discord states. Interpreting the Werner states, isotropic states and some of the \( X \) states as graph Laplacian states, we derive its discord.

The article is organized as follows. We provide a brief overview of graph theory which is required for the remaining part of the article. We establish the condition for a quantum state to be a graph Laplacian state. In Section 3, we establish the condition on clusters of a weighted directed graph such that the blocks of the corresponding graph Laplacian states form a family of commuting normal matrices. In the next section, we combine these results to generate the graph theoretic criterion of zero discord. Finally we employ these results on some
well known states, for example, Werner, Isotropic, and the X states. We then conclude.

2 Preliminaries

A weighted digraph is an ordered pair of sets denoted by $G = (V(G), E(G))$ where $V(G)$ is called the vertex set and $E(G) \subseteq V \times V$ a set of ordered pair of vertices called the edge set with a weight function $w_G : E(G) \to \mathbb{C} \setminus \{0\}$ [7]. If there is no confusion regarding the underlined digraph $G$, we simply denote $w$ for $w_G$. Now, we consider the following assumptions on all weighted digraphs considered in the article.

Assumptions:

1. Given two vertices $i$ and $j$, if $(i, j) \in E(G)$ then $(j, i) \in E(G)$ and $w(j, i) = \overline{w(i, j)}$, the complex conjugate of $w(i, j)$.

2. If $(i, i) \in E(G)$ then $w(i, i) \in \mathbb{R}$, the set of real numbers.

Note that if $w(i, j) = 1$ for all $(i, j) \in E(G)$ and $(i, i) \notin E(G)$ for all $i \in V(G)$ then the digraph $G$ becomes a simple graph. Let $G$ be a weighted digraph on $N$ vertices. Then the adjacency matrix $A(G) = [a_{ij}]_{N \times N}$ associated with a weighted digraph $G$ is defined by,

$$a_{ij} = \begin{cases} w(i, j) & \text{if } (i, j) \in E(G), \\ 0 & \text{if } (i, j) \notin E(G) \end{cases}$$

and $a_{ji} = \overline{a_{ij}} = \overline{w(i, j)}$. Thus $A(G)$ is a Hermitian matrix. The weighted degree of a vertex $i$ is defined by

$$d_i = \sum_{(i, j) \in E(G)} |w(i, j)| = \sum_{j=1}^{N} |a_{i,j}|.$$  \hfill (2)

The degree matrix is the diagonal matrix is defined by $D(G) = \text{diag}\{d_1, d_2, \ldots, d_N\}$. The Laplacian and the signless Laplacian matrices are defined by $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$, respectively. It is proved in [7] that $L(G)$ and $Q(G)$ are positive semidefinite Hermitian matrices. Recall that a density matrix $\rho$ corresponding to a quantum state is a positive semi-definite Hermitian matrix with unit trace. Consequently the density matrices corresponding to a weighted digraph are defined as

$$\rho_l(G) = \frac{1}{\text{trace}(L(G))}L(G) \quad \text{and} \quad \rho_q(G) = \frac{1}{\text{trace}(Q(G))}Q(G).$$ \hfill (3)

We denote $\rho_l(G)$ and $\rho_q(G)$ together with $\rho(G)$ when no confusion arises. We call the digraph $G$ as the graph representation of $\rho(G)$. Then we have the following lemma.
Lemma 1. A density matrix $\rho = (\rho_{ij})_{N \times N}$ has a graph representation if and only if for all $i$ and $j$, $\rho_{ii} \geq \sum_{i \neq j} |\rho_{ij}|$.

Proof. If $\rho$ has a graph representation, the weighted digraph $G$ has $N$ vertices since the order of $\rho$ is $N$. When $i \neq j$ and $\rho_{ij} \neq 0$ there is a directed edge $(i, j)$ with edge weight $w(i, j) = \rho_{ij}$. As $\rho$ is a positive semi-definite Hermitian matrix, $\rho_{ji} = \overline{\rho_{ij}}$ and $\rho_{ii}$ is a non-negative real number. Thus $(i, j)$ and $(j, i)$ exist together with $w(j, i) = w(i, j)$. Besides, $\rho_{ii} = d_i + sa_{ii}$. Here $s = -1$ for $\rho_l(G)$ and $s = 1$ for $\rho_q(G)$. Now,

$$
\rho_{ii} = d_i + sa_{ii} = \sum_{j=1}^{N} |w(i, j)| + sw(i, i) = \sum_{j \neq i} |w(i, j)| + |w(i, i)| + sw(i, i) 
$$

As $\rho_{ii}$ is real, $w(i, i)$ must be real in the above expression. Now two cases arise.

- Case-I: Let $w(i, i) = 0$ or $|w(i, i)| = -sw(i, i)$. In any case, $\rho_{ii} = \sum_{j \neq i} |\rho_{ij}|$.
- Case-II: Let $w(i, i) \neq 0$ and $|w(i, i)| + sw(i, i) = 2|w(i, i)|$. Then, from the above equation,

$$
|w(i, i)| = \frac{\rho_{ii} - \sum_{i \neq j} |\rho_{ij}|}{2} \geq 0. 
$$

In this case, $\rho_{ii} \geq \sum_{i \neq j} |\rho_{ij}|$.

Now we state the following definition and examples.

Definition 1. Graph Laplacian quantum states: A quantum state $\rho$ is said to be a graph Laplacian state if there exist a weighted directed graph $G$ such that $\rho = \rho(G)$.

Note that any graph Laplacian state satisfies Lemma 1.

Example 1. Consider the quantum state

$$
\rho = \frac{1}{5} |0\rangle \langle 0| + \frac{2}{5} |0\rangle \langle 1| + \frac{2}{5} |1\rangle \langle 0| + \frac{4}{5} |1\rangle \langle 1| = \frac{1}{5} \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}.
$$

Note that, $\rho_{11} \leq \rho_{12}$. Thus, this quantum state is not graphical.

From now onwards we use the word graph for weighted directed graph. The following describes the framework for interpreting any graph $G$ on $mn$ vertices as a graph with $m$ clusters each with $n$ vertices. Recall that cluster of a graph
is a subgraph of the graph. Consider a partition of the vertex set $V(G)$ that produces these clusters as follows.

$$V = C_1 \cup C_2 \cup \cdots \cup C_m;$$

$$C_\mu \cap C_\nu = \emptyset \text{ for } \mu \neq \nu \text{ and } \mu, \nu = 1, 2, \ldots m;$$

$$C_\mu = \{v_{\mu_1}, v_{\mu_2}, \ldots v_{\mu_n}\}.$$ 

For any vertex $v_{\gamma i}$, the Roman index $i$ represents the position of a vertex in $\gamma$-th cluster indexed by a Greek index. Then

$$A(G) = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & A_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mm} \end{bmatrix}_{m \times m},$$

where $A_{\mu \nu}$ are blocks of order $n \times n$ [18]. As $A(G)$ is a Hermitian matrix, we have $A^\dagger_{\mu \nu} = A_{\mu \nu}$ and $A^\dagger_{\nu \mu} = A_{\nu \mu}$, for $\mu \neq \nu$. Now we recall the definition of induced subgraph [19].

**Definition 2. Induced Subdigraph:** A subdigraph $H$ of a digraph $G$ is an induced subdigraph if $u, v \in V(H)$ and $(u, v) \in E(G)$ implies $(u, v) \in E(H)$.

We denote the induced subdigraph generated by the cluster $C_\mu$ by $(C_\mu)$. Also the subdigraph $(C_\mu, C_\nu)$ consists of all the vertices in $C_\mu \cup C_\nu$, and all the edges $(u, v)$ and $(v, u)$ with $u \in C_\mu$, and $v \in C_\nu$. In the equation (7), the block $A_{\mu \nu}$ acts as the adjacency matrix of the cluster $C_\mu$. Further, $A_{\mu \nu}$ represents all the edges joining two vertices belonging to different clusters $C_\mu$ and $C_\nu$. Thus,

$$A((C_\mu, C_\nu)) = \begin{bmatrix} 0 & A_{\mu \nu} \\ A_{\nu \mu} & 0 \end{bmatrix} = \begin{bmatrix} 0 & A_{\mu \nu}^\dagger \\ A_{\mu \nu} & 0 \end{bmatrix}. \quad (8)$$

This clustering on $V(G)$ also partitions the degree matrix into blocks, such that, $D = \text{diag}\{D_1, D_2, \ldots D_m\}$, where $D_\mu$ is a diagonal matrix containing degree of the vertices in $C_\mu$. If $B_{\mu \nu}$ are blocks of the density matrix $\rho(G)$, then

$$B_{\mu \nu} = \begin{cases} A_{\mu \nu} / d & \text{if } \mu \neq \nu \\ D_{\mu \nu} + \lambda A_{\mu \mu} / d & \text{if } \mu = \nu \end{cases}, \quad (9)$$

where $s = 1$ and $-1$ for $\rho(G) = \rho_q(G)$ and $\rho_l(G)$ respectively.

A bipartite density matrix acts on the Hilbert space $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)}$ where $\mathcal{H}^{(A)}$ and $\mathcal{H}^{(B)}$ denote the state spaces (Hilbert spaces) corresponding to the constituent systems $A$ and $B$ respectively, $\otimes$ denotes the Kronecker (tensor) product. For any bipartite density matrix $\rho$, there are two reduced density matrices $\rho_a$ and $\rho_b$ acting on the spaces $\mathcal{H}^{(A)}$ and $\mathcal{H}^{(B)}$, respectively. The mutual information in $\rho$ is defined as $I(\rho) = S(\rho_a) + S(\rho_b) - S(\rho)$ where $S(X) = -\text{trace}(X \log(X))$ is the von-Neumann entropy of a state $X$. Let the set of all possible von Neumann measurements with respect to the system
Thus we obtain another measure of mutual information in $\rho$ given by $I(\rho|\Pi^b) = S(\rho_a) - S(\rho|\Pi^b)$, where $S(\rho|\Pi^b) = \sum_k p_k S(\rho_k)$, and $p_k = \frac{1}{\dim(H^b)}(I_a \otimes \Pi^b_k) \rho (I_a \otimes \Pi^b_k) \rho (I_a \otimes \Pi^b_k)$, with $p_k = \text{trace}(I_a \otimes \Pi^b_k) \rho (I_a \otimes \Pi^b_k)$, $k = 1, 2, \ldots \dim(H^b)$. Quantum discord is the difference between these two classically equivalent measures $I(\rho)$ and $I(\rho|\Pi^b)$ [11, 10]. There are quantum states which yield equal value for both the measures that are known as classical-quantum states [20] or pointer states.

**Definition 3. Quantum discord:** The quantum discord of a bipartite state $\rho$ is

$$D(\rho) = \min_{\Pi^b} \{ I(\rho) - I(\rho|\Pi^b) \}. \quad (10)$$

Here, we consider the canonical computational basis $\{|i_a\rangle\}$ of $\mathcal{H}^{(A)}$, and $\{|i_b\rangle\}$ of $\mathcal{H}^{(B)}$. We can express $\rho$ as,

$$\rho = \sum_{i,j} E_{ij} \otimes B_{ij}, \quad (11)$$

where, $E_{ij} = |i_a\rangle \langle j_a|$, and $B_{i,j} = \text{trace}_a([|j_a\rangle \langle i_a| \otimes I_b] \rho)$. Thus, $B_{ij}$ are blocks of the density matrix $\rho$ and has zero discord if and only if $\{B_{ij}\}$ is a family of commuting normal matrices [16].

**3 Graph theoretic perspective of a family of normal commuting matrices**

In this section we find graph theoretic conditions for normal and commuting matrices in terms of subgraphs generated with clustering on the vertex set. These conditions are based on the neighborhood of individual vertices in the considered subgraphs.

Given a vertex $i$ we call the set $\text{nbd}_G(i) = \{ j : j \in V(G), (i,j) \in E(G) \}$ as the neighborhood of vertex $i$. Under the basic assumptions outlined above, $(i,j)$ and $(j,i)$ belong to $E(G)$ together. With respect to the vertex $i$ we describe $(i,j)$ as the outgoing edge and $(j,i)$ as the incoming edge. We collect the weights of the edges incident to vertex $i$ in the following sets.

$$W(\text{nbd}_G(i)_{out}) = \{ w_G(i,j) : (i,j) \in E(G) \},$$

$$W(\text{nbd}_G(i)_{in}) = \{ w_G(j,i) : (j,i) \in E(G) \}. \quad (12)$$

**Definition 4. Support of a vector:** Given a vector $a \in \mathbb{C}^n$ there is a set $\text{nbd}(a)$ defined by,

$$\text{nbd}(a) = \{ i : a(i) \neq 0 \}$$

where $a(i)$ denotes the $i$th entry of $a$.

Given two vectors $a,b \in \mathbb{C}^n$ we define their product as,

$$\langle a, b \rangle = \sum_{k \in \text{nbd}(a) \cap \text{nbd}(b)} a(k)b(k). \quad (13)$$
Given a matrix \( A = (a_{ij})_{n \times n} \), \( a_{is} \) and \( a_{sj} \) denotes the \( i \)-th row and \( j \)-th column vectors, respectively. Corresponding to every \( A \), there is a weighted bipartite graph of order 2\( n \), \( \mathcal{A} = (V(\mathcal{A}), E(\mathcal{A})) \) with the adjacency matrix,

\[
A(\mathcal{A}) = \begin{bmatrix} 0 & A \\ A^\dagger & 0 \end{bmatrix}.
\]  

(14)

As \( \mathcal{A} \) is a bipartite graph we can write \( V(\mathcal{A}) = C_\mu \cup C_\nu \), where \( C_\mu = \{v_{\mu 1}, v_{\mu 2}, \ldots, v_{\mu n}\} \), \( C_\nu = \{v_{\nu 1}, v_{\nu 2}, \ldots, v_{\nu n}\} \) and \( C_\mu \cap C_\nu = \emptyset \) as mentioned in equation (6). Therefore, \( \mathcal{A} = (C_\mu, C_\nu) \), the subgraph generated by the vertex sets \( C_\mu \) and \( C_\nu \). The directed edge \((v_{\mu i}, v_{\nu j}) \in E(\mathcal{A})\), if and only if \( a_{ij} \neq 0 \). Also, \( w(v_{\mu i}, v_{\nu j}) = a_{ij} \). Moreover, the adjacency matrix \( A(\mathcal{A}) \) indicates the existence of \((v_{\nu j}, v_{\mu i})\) with \( w(v_{\nu j}, v_{\mu i}) = \overline{a}_{ij} \). Now,

\[
\text{nbd}_\mathcal{A}(v_{\mu i}) = \{v_{\nu j} : (v_{\mu i}, v_{\nu j}) \in E(G)\} \subset C_\nu.
\]  

(15)

Similarly, \( \text{nbd}_\mathcal{A}(v_{\nu i}) \subset C_\mu \). Let \( 0_{1,n} \) and \( 0_{n,1} \) are zero row and column vectors. Note that, the \( i \)-th row of \( A(\mathcal{A}) \), that is \((0_{1,n}, a_{is})\) represents weights of outgoing edges from the vertex \( v_{\nu i} \). According to the definition 4, \( \text{nbd}(0_{1,n}, a_{is}) = \text{nbd}(a_{is}) \) which represents indexes of vertices in \( \text{nbd}_\mathcal{A}(v_{\mu i}) \). Thus we have,

\[
\text{nbd}(a_{is}) = \text{nbd}_\mathcal{A}(v_{\mu i}), \text{ and } a_{is} = W(\text{nbd}_\mathcal{A}(v_{\mu i}))_{\text{out}}.
\]  

(16)

Similarly, the \((n + i)\)-th column of \( A(\mathcal{A}) \), that is \((a_{si}, 0_{n,1})\) represents edge weights of the incoming edges to the vertex \( v_{\nu i} \). Also, \( \text{nbd}(a_{si}) \) represents indexes of vertices in \( \text{nbd}_\mathcal{A}(v_{\nu i}) \). Hence,

\[
\text{nbd}(a_{si}) = \text{nbd}_\mathcal{A}(v_{\nu i}) \text{ and } a_{si} = W(\text{nbd}_\mathcal{A}(v_{\nu i}))_{\text{in}}.
\]  

(17)

In particular, any complex Hermitian matrix \( A \) of order \( n \) can be considered as an adjacency matrix of a graph \( \tilde{\mathcal{A}} \), where \( V(\tilde{\mathcal{A}}) = C_\mu = \{v_{\mu 1}, v_{\mu 2}, \ldots, v_{\mu n}\} \). The edge \((v_{\mu i}, v_{\nu j}) \in E(\tilde{\mathcal{A}})\) if and only if \( a_{ij} \neq 0 \). Thus, \( \tilde{\mathcal{A}} = (C_\mu) \), the induced subgraph generated by the vertex set \( C_\mu \). Here, the row vector \( a_{is} \) represents all outgoing edges from the vertex \( v_{\mu i} \). Thus, \( \text{nbd}(a_{is}) = \text{nbd}_{\tilde{\mathcal{A}}}(v_{\mu i}) \). Similarly, \( \text{nbd}(a_{si}) = \text{nbd}_{\tilde{\mathcal{A}}}(v_{\nu i}) \).

**Lemma 2.** Let the weighted bipartite digraphs corresponding to complex square matrices \( A \) and \( B \) of order \( n \) be \( \mathcal{A} = (C_\mu, C_\nu) \), and \( \mathcal{B} = (C_\alpha, C_\beta) \), respectively. The matrices \( A \) and \( B \) commute, if and only if for all \( i, j \) with \( 1 \leq i, j \leq n \),

\[
\sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\nu k}) w(v_{\nu k}, v_{\beta j}) = \sum_{k \in \text{nbd}(v_{\alpha i}) \cap \text{nbd}(v_{\nu j})} w(v_{\alpha i}, v_{\beta k}) w(v_{\beta k}, v_{\nu j}).
\]

Proof. Commutativity \( AB = BA \) holds if and only if \((AB)_{ij} = (BA)_{ij}\) for all \( i, j \) with \( 1 \leq i, j \leq n \). Note that, \( a_{ik} = w(v_{\mu i}, v_{\nu k}) \) and \( b_{kj} = w(v_{\nu k}, v_{\beta j}) \). Now
Lemma 3. Let \( A = (a_{ij})_{n \times n} \) be a weighted bipartite digraph corresponding to a matrix \( A = (a_{ij})_{n \times n} \). It is normal, if and only if for every \( i, j \) with \( 1 \leq i, j \leq n \),

\[
\sum_{k \in \text{nbd}(v_{ui}) \cap \text{nbd}(v_{uj})} w(v_{ui}, v_{uk})w(v_{uk}, v_{uj}) = \sum_{k \in \text{nbd}(v_{ui}) \cap \text{nbd}(v_{uj})} w(v_{ui}, v_{uk})w(v_{uk}, v_{uj}).
\]

Note that, if \( \langle C_\mu, C_\nu \rangle = \langle C_\alpha, C_\beta \rangle \) then the condition of commutativity holds. Also, if any of the graphs be empty, then the commutativity condition holds trivially.

Corollary 1. Let \( \hat{A} = (C_\mu) \), and \( B = (C_\alpha, C_\beta) \) be graphs corresponding to a Hermitian matrix \( A = (a_{ij})_{n \times n} \), and square matrix \( B = (b_{ij})_{n \times n} \). They commute if and only if for all \( i, j \) with \( 1 \leq i, j \leq n \),

\[
\sum_{k \in \text{nbd}(v_{ui}) \cap \text{nbd}(v_{uj})} w(v_{ui}, v_{uk})w(v_{uk}, v_{uj}) = \sum_{k \in \text{nbd}(v_{ui}) \cap \text{nbd}(v_{uj})} w(v_{ui}, v_{uk})w(v_{uk}, v_{uj}).
\]

Proof. We have already justified that, \( \text{nbd}(a_{is}) = \text{nbd}(\hat{A})(v_{is}) \) and \( \text{nbd}(a_{js}) = \text{nbd}(\hat{A})(v_{js}) \), for all \( i = 1, 2, \ldots n \). The matrix \( A \) commutes with \( B \), if and only if the product \( \langle a_{is}, b_{js} \rangle = \langle b_{is}, a_{js} \rangle \) for all \( i, j \). Applying the symmetry of \( A \), we get, \( \langle a_{is}, b_{js} \rangle = \langle a_{js}, b_{is} \rangle \). Using the graph theoretic convention, we get the desired result.

Corollary 2. Two Hermitian matrices \( A = (a_{ij})_{n \times n} \), and \( B = (b_{ij})_{n \times n} \) corresponding to graphs \( \hat{A} = (C_\mu) \), and \( \hat{B} = (C_\nu) \) commute, if and only if for every \( i, j \) with \( 1 \leq i, j \leq n \),

\[
\sum_{k \in \text{nbd}(v_{ui}) \cap \text{nbd}(v_{uj})} w(v_{ui}, v_{uk})w(v_{uk}, v_{uj}) = \sum_{k \in \text{nbd}(v_{ui}) \cap \text{nbd}(v_{uj})} w(v_{ui}, v_{uk})w(v_{uk}, v_{uj}).
\]

Proof. The proof follows from the above Corollary by choosing \( \alpha = \beta = \nu \).

A complex normal matrix \( A \) commutes with its conjugate transpose, that is \( AA^\dagger = A^\dagger A \). Hermitian matrices are trivially normal matrices. But there are normal matrices which are not Hermitian.

Lemma 3. Let \( A = (C_\mu, C_\nu) \) be a weighted bipartite digraph corresponding to a matrix \( A = (a_{ij})_{n \times n} \). It is normal, if and only if for every \( i, j \) with \( 1 \leq i, j \leq n \),

\[
\sum_{k \in \text{nbd}(v_{ui}) \cap \text{nbd}(v_{uj})} w(v_{ui}, v_{uk})w(v_{uk}, v_{uj}) = \sum_{k \in \text{nbd}(v_{ui}) \cap \text{nbd}(v_{uj})} w(v_{ui}, v_{uk})w(v_{uk}, v_{uj}).
\]
Proof. Let $B = (b_{ij})_{n \times n} = (a_{ji})_{n \times n} = A^\dagger$. Clearly, $b_{is} = a_{is}^\dagger$ and $b_{si} = a_{si}^\dagger$ for all $i$. Note that,
\[
(AA^\dagger)_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj} = \langle a_{is}, b_{sj} \rangle = \langle a_{is}, a_{js} \rangle
\]
\[
= \sum_{k} w(v_{\mu i}, v_{\nu k}) w(v_{\nu k}, v_{\mu j}) : k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\mu j}).
\]
Similarly, $(A^\dagger A)_{ij} = \sum_{k} w(v_{\nu i}, v_{\mu k}) w(v_{\mu k}, v_{\nu j}) : k \in \text{nbd}(v_{\nu i}) \cap \text{nbd}(v_{\nu j})$.
Hence, we get the equality as stated for normality. \qed

Now we consider a trivial observation related to the above lemma, which will be used later. Let there be only one edge of arbitrary non-zero weight, $(v_{\mu p}, v_{\nu q})$ with $p \neq q$, between two clusters $C_\mu$ and $C_\nu$. Now, for $i = j = p$,
\[
\sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\nu k}) w(v_{\nu k}, v_{\mu j}) = w(v_{\mu p}, v_{\nu q}) w(v_{\nu q}, v_{\mu pp}).
\]
Also, for $i = j = p$ the set $\text{nbd}(v_{\mu j}) \cap \text{nbd}(v_{\nu j}) = \emptyset$, as $v_{\mu p}$ is an isolated vertex. Hence, the term $\sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\nu k}) w(v_{\nu k}, v_{\mu j})$ takes no value. In this case, the graph $\langle C_\mu, C_\nu \rangle$ fails to fulfill the normality condition. Note that, for $p = q$ the graph $\langle C_\mu, C_\nu \rangle$ with single edge $(v_{\mu p}, v_{\nu q})$ represents a normal matrix.

4 Graph theoretic condition of zero discord

Let us recollect some important facts discussed in the earlier sections. The Lemma 1 provides conditions on a quantum state $\rho$ acting on $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$ to have a graph representation. In the equation (6), we partition a digraph with $N = mn$ vertices into clusters. Thus two sets of subgraphs are generated: \{\langle C_\mu \rangle : \mu = 1, 2, \ldots, m\} where every graph is of order $n$, and \{\langle C_\mu, C_\nu \rangle : \mu, \nu = 1, 2, \ldots, m; \mu \neq \nu\} where every graph is bipartite graph with $2n$ vertices. We have discussed forms of the adjacency matrices $A(\langle C_\mu, C_\nu \rangle)$ and $A(\langle C_\mu \rangle)$ in the last section. Commutativity condition of two matrices $A$ and $B$ were discussed in terms of digraphs $\langle C_\mu, C_\nu \rangle$ and $\langle C_\mu \rangle$ in the lemma 2, and its corollaries 1 and 2. That the matrix $A$ normal has been discussed in the lemma 3. Hence, if the blocks of a given graphical density matrix form a family of commuting normal matrices, the underlined graph will satisfy all these graphical conditions. We combine them in the following theorem.

Theorem 1. Blocks of a density matrix $\rho$ acting on $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$ form a family of commuting normal matrices if and only if the following conditions are satisfied.

1. Commutativity condition: Given any two subgraphs $\langle C_\mu, C_\nu \rangle$, and $\langle C_\alpha, C_\beta \rangle$ and for all $i, j$ with $1 \leq i, j \leq n$,
\[
\sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\nu k}) w(v_{\nu k}, v_{\mu j}) = \sum_{k \in \text{nbd}(v_{\alpha i}) \cap \text{nbd}(v_{\beta j})} w(v_{\alpha i}, v_{\beta k}) w(v_{\beta k}, v_{\alpha j}).
\]
2. **Normality condition:** For all subgraph \((C_\mu, C_\nu)\) and for every \(i, j\) with \(1 \leq i, j \leq n\),
\[
\sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\nu k})w(v_{\nu k}v_{\mu j}) = \sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\nu i}, v_{\mu k})w(v_{\mu k}v_{\nu j}).
\]

3. **Degree condition** The graph satisfies the following two degree criterion,
\[
(a) \\
\pm \left[w(v_{\mu i}, v_{\mu j})(d_{\mu i} - d_{\mu j}) + w(v_{\mu i}, v_{\nu j})(d_{\nu j} - d_{\nu i})\right] + \sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\nu k})w(v_{\nu k}v_{\mu j}) \Rightarrow \sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\nu i}, v_{\mu k})w(v_{\mu k}v_{\nu j}) = 0,
\]
\[
(b) \\
w(v_{\alpha i}, v_{\beta j})(d_{\mu i} - d_{\mu j}) \pm \sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\beta j})} w(v_{\mu i}, v_{\nu k})w(v_{\nu k}v_{\beta j}) - \sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\beta j})} w(v_{\alpha i}, v_{\beta j})w(v_{\beta j}v_{\mu j}) = 0.
\]

**Proof.** The commutativity and normality conditions follow from the lemma 2 and 3 for all non-diagonal blocks. Note that, diagonal blocks are adjacency matrices of \((C_\mu)\) which are Hermitian, hence normal. The degree condition includes all diagonal blocks in this family.

First we consider commutativity of two diagonal blocks,
\[
\frac{1}{d}(D_\mu \pm A_{\mu \mu}) \frac{1}{d}(D_\nu \pm A_{\nu \nu}) = \frac{1}{d}(D_\nu \pm A_{\nu \nu}) \frac{1}{d}(D_\mu \pm A_{\mu \mu}) \\
\Rightarrow D_\mu D_\nu \pm D_\mu A_{\nu \nu} \pm A_{\mu \mu} D_\nu = D_\nu D_\mu \pm D_\nu A_{\mu \mu} \pm A_{\nu \nu} A_{\mu \mu} \\
\Rightarrow (A_{\mu \mu} A_{\nu \nu} - A_{\nu \nu} A_{\mu \mu}) \pm (D_\mu A_{\nu \nu} - A_{\nu \nu} D_\mu) \pm (A_{\mu \mu} D_\nu - D_\nu A_{\mu \mu}) = 0 \\
\Rightarrow (A_{\mu \mu} A_{\nu \nu} - A_{\nu \nu} A_{\mu \mu})_{ij} \pm (D_\mu A_{\nu \nu} - A_{\nu \nu} D_\mu)_{ij} \pm (A_{\mu \mu} D_\nu - D_\nu A_{\mu \mu})_{ij} = 0.
\]

In terms of graphical parameters we may write,
\[
(D_\mu A_{\nu \nu} - A_{\nu \nu} D_\mu)_{ij} = d_{\mu i}(A_{\nu \nu})_{ij} - (A_{\nu \nu})_{ij}d_{\mu j} = w(v_{\mu i}, v_{\nu j})(d_{\mu i} - d_{\mu j}), \quad (24) \\
(A_{\mu \mu} D_\nu - D_\nu A_{\mu \mu})_{ij} = (A_{\mu \mu})_{ij}d_{\nu j} - d_{\nu i}(A_{\nu \nu})_{ij} = w(v_{\mu i}, v_{\nu j})(d_{\nu j} - d_{\nu i}). \quad (25)
\]

Also from the corollary 2,
\[
(A_{\mu \mu} A_{\nu \nu} - A_{\nu \nu} A_{\mu \mu})_{ij} = \\
\sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\nu k})w(v_{\nu k}v_{\nu j}) - \sum_{k \in \text{nbd}(v_{\nu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\nu i}, v_{\nu k})w(v_{\mu k}v_{\nu j}). \quad (26)
\]
Thus for commutativity of diagonal blocks the following degree condition need to be satisfied,
\[
\sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\mu k})w(v_{\nu k}, v_{\nu j}) - \sum_{k \in \text{nbd}(v_{\nu i}) \cap \text{nbd}(v_{\mu j})} w(v_{\mu i}, v_{\nu k})w(v_{\mu k}, v_{\nu j}) \\
\pm [w(v_{\mu i}, v_{\nu j})(d_{\mu i} - d_{\mu j}) + w(v_{\mu i}, v_{\nu j})(d_{\nu j} - d_{\nu i})] = 0.
\]
\(27\)

We consider + for \(\rho_q(G)\) and − for \(\rho_l(G)\) in the above equation.

Now we consider commutativity of a diagonal and a non-diagonal block.
\[
\frac{1}{d}(D_{\mu} \pm A_{\mu\mu}) \frac{1}{d}A_{\alpha\beta} = \frac{\pm 1}{d}A_{\alpha\beta} \frac{1}{d}(D_{\mu} \pm A_{\mu\mu}) \\
\Rightarrow D_{\alpha\beta} \pm A_{\mu\mu}A_{\alpha\beta} = A_{\alpha\beta}D_{\mu} \pm A_{\alpha\beta}A_{\mu\mu}.
\]
\(28\)

Rearranging the terms we get the equation,
\[
(D_{\mu}A_{\alpha\beta} - A_{\alpha\beta}D_{\mu}) \pm (A_{\mu\mu}A_{\alpha\beta} - A_{\alpha\beta}A_{\mu\mu}) = 0.
\]
\(29\)

The above equation holds if for all \(i, j\) with \(1 \leq i, j \leq n\),
\[
(D_{\mu}A_{\alpha\beta})_{ij} - (A_{\alpha\beta}D_{\mu})_{ij} \pm \{(A_{\mu\mu}A_{\alpha\beta})_{ij} - (A_{\alpha\beta}A_{\mu\mu})_{ij}\} = 0
\]
\(30\)

Graph theoretic counterpart of \((A_{\mu\mu}A_{\alpha\beta} - A_{\alpha\beta}A_{\mu\mu})\) follows from the corollary 1. Thus,
\[
(A_{\mu\mu}A_{\alpha\beta})_{ij} - (A_{\alpha\beta}A_{\mu\mu})_{ij} = \\
\sum_{k \in \text{nbd}(v_{\alpha i}) \cap \text{nbd}(v_{\beta j})} w(v_{\mu i}, v_{\mu k})w(v_{\alpha k}, v_{\beta j}) - \sum_{k \in \text{nbd}(v_{\alpha i}) \cap \text{nbd}(v_{\beta j})} w(v_{\alpha i}, v_{\beta k})w(v_{\mu k}, v_{\beta j}).
\]
\(31\)

Also,
\[
d_{\mu i}(A_{\alpha\beta})_{ij} - (A_{\alpha\beta})_{ij}d_{\mu j} = w(v_{\alpha i}, v_{\beta j})(d_{\mu i} - d_{\mu j}).
\]
\(32\)

Combining the above two equations we get,
\[
w(v_{\alpha i}, v_{\beta j})(d_{\mu i} - d_{\mu j}) \pm \left[ \sum_{k \in \text{nbd}(v_{\alpha i}) \cap \text{nbd}(v_{\beta j})} w(v_{\mu i}, v_{\mu k})w(v_{\alpha k}, v_{\beta j}) - \sum_{k \in \text{nbd}(v_{\alpha i}) \cap \text{nbd}(v_{\beta j})} w(v_{\alpha i}, v_{\beta k})w(v_{\mu k}, v_{\beta j}) \right] = 0.
\]
\(33\)

Now we have several observations. If vertices of \(C_\mu, \mu = 1, 2, \ldots m\) have equal degree, then \(d_{\mu i} - d_{\mu j} = 0\) independent of the existence of edge \((v_{\alpha i}, v_{\beta j})\).
In this case, the graph satisfies the Property 4 if every pair of subgraph \( \langle C_\mu \rangle \) and \( \langle C_\alpha, C_\beta \rangle \) satisfies the Corollary 1.

Also if the subgraphs \( \langle C_\mu \rangle \) and \( \langle C_\nu \rangle \) fulfill the commutativity condition described in the corollary 2 then the first degree condition takes the following simpler form:

\[
w(v_{\alpha i}, v_{\nu j})(d_{\mu i} - d_{\mu j}) + w(v_{\mu i}, v_{\nu j})(d_{\nu j} - d_{\nu i}) = 0 \text{ for all } i,j.
\]  \( (34) \)

Further, if the subgraphs \( \langle C_\alpha, C_\beta \rangle \) and \( \langle C_\mu \rangle \) satisfy the commutativity condition described in the corollary 1 the equation is simplified to

\[
w(v_{\alpha i}, v_{\beta j})(d_{\mu i} - d_{\mu j}) = 0 \text{ for all } i,j.
\]  \( (35) \)

When the graph is a simple graph, \( w(u, v) = 1 \) for all \( (u, v) \in E(G) \). Then this conditions on weighted graphs are consistent with that of simple graphs discussed in [8].

5 Discord of some graph Laplacian states

In this section, we study three classes of mixed quantum states: the Werner, isotropic, and the \( X \) states of arbitrary dimensions. We show when these can be represented as graph Laplacian states. Using the results of the earlier sections we obtain graph theoretic conditions for these states to have zero quantum discord.

5.1 Werner state

A Werner state [21] is represented by,

\[
\rho_{x,d} = \frac{d - x}{d^3 - d} I + \frac{xd - 1}{d^3 - d} F,
\]  \( (36) \)

where \( F = \sum_{i,j} |i\rangle \langle j| \otimes |j\rangle \langle i|, x \in [0, 1] \) and \( d \) is the dimension of the individual subsystems. Note that, \( \rho_{x,d} \) is a real symmetric matrix of order \( d^2 \). These are separable Werner states with non-zero quantum discord [22].

We show that all the Werner states are graph Laplacian states. As \( \rho_{x,d} \) acts on the space \( \mathcal{H}(d) \otimes \mathcal{H}(d) \), we partition the vertex set into \( d \) clusters \( C_\mu, \mu = 1, 2, \ldots, d \), each having \( d \) vertices. The corresponding digraph has three types of edges:

1. Loops at diagonal vertices \( v_{11}, v_{22}, \ldots, v_{dd} \) having loop weights \( w(v_{\mu,\mu}, v_{\mu,\mu}) = (d - 1) + (d - 1)x \).
2. Loops at non-diagonal vertices \( \{v_{\mu,i} : \mu \neq i\} \) having loop weights \( w(v_{\mu,i}, v_{\mu,i}) = d - x \).
3. Non-loop edges with weight \( w(v_{\mu,i}, v_{i,\mu}) = dx - 1 \). Note that, there is only one edge between two different clusters. All such edges are diagonal and parallel to each-other.
The following example would help to illustrate this structure.

**Example 2.** We may represent $\rho_{x,3}$ and $\rho_{x,4}$ as a graph with 9 and 16 vertices depicted in figure 1. The edge weights $a, b$, and $c$ represent weights of different classes of edges discussed above.

**Theorem 2.** Graph Laplacian Werner states have non-zero quantum discord except some specific values of $x$.

**Proof.** Note that, for all $x$ there is only an edge $(v_{i,i}, v_{i,j})$ in the subgraph $\langle C_\mu, C_i \rangle$ where $\mu \neq i$. After the lemma 3 we have shown such type of graphs cannot fulfill normality condition.

As an example, consider the subdigraph $\langle C_1, C_2 \rangle$ of $\rho_{x,3}$ depicted in figure 2. There is only one edge $(v_{1,2}, v_{2,1})$ with weight $(3x - 1)$ between two clusters $C_1$ and $C_2$. The edge weight is non-zero when $x \neq \frac{1}{3}$. Note that, $w(v_{12}, v_{21})w(v_{21}, v_{12}) = (3x - 1)^2$ but $w(v_{22}, v_{12})w(v_{12}, v_{12}) = 0$ as $v_{22}$ is an isolated vertex. In this case, the graph $\langle C_1, C_2 \rangle$ fulfills the normality condition if and only if $x = \frac{1}{3}$.

Thus the normality condition of the theorem 1 is violated except some parameter values. Hence, graph Laplacian Werner states have non-zero quantum discord except some specific values of $x$. \qed
5.2 Isotropic state

An isotropic state $\rho_{d,x}$ acting on $H^{(d)} \otimes H^{(d)}$ is defined by,

$$\rho_{d,x} = \frac{d^2}{d^2 - 1} \left[ \frac{(1 - F)}{d^2} I + \left( F - \frac{1}{d^2} \right) P \right],$$

where $F \in [0, 1]$ is the fidelity of the quantum state and $P = \langle \psi | \psi \rangle$ where $|\psi\rangle = \frac{1}{\sqrt{d}} \sum_i |i_a\rangle |i_b\rangle$, the maximally entangled state in dimension $d$. Discord of isotropic state is studied in [23, 24]. Considering diagonal and off-diagonal terms we may conclude that an isotropic quantum state is graphical provided

$$(d - 1) \left| F - \frac{1}{d^2} \right| \leq \frac{d^2 - 1}{d^2} F.$$  

Putting $d = 2, 3, 4$ in the above equation we get, $\frac{1}{4} \leq F \leq 1$, $\frac{1}{13} \leq F \leq \frac{1}{9}$, $\frac{1}{11} \leq F \leq \frac{1}{27}$, respectively.

As $\rho_{d,x}$ acts on $H^{(d)} \otimes H^{(d)}$, we represent the vertex set into $d$ clusters $C_\mu : \mu = 1, 2, \ldots d$ with $C_\mu = \{v_{\mu 1}, v_{\mu 2}, \ldots v_{\mu n}\}$. We observe that a graph representing an isotropic state has the following properties.

1. The diagonal vertices $v_{1 1}, v_{2 2}, \ldots v_{dd}$ form a complete graph which consists of all non-loop edges of the graph. Weight of these edges are $F - \frac{1}{d^2}$.

2. The loop weight of the non-diagonal vertices is $\frac{1}{d^2} F$.

3. The loop weight of the diagonal vertices are given by $\frac{d^2 - 1}{d^2} F$.

**Example 3.** Graph representations of the isotropic state $\rho_{d,x}$ for $d = 2, 3, 4$ are depicted in the figure 3. In the picture, all the edges and loops are weighted as described above.

**Theorem 3.** Graph Laplacian isotropic states have non-zero quantum discord except for some specific values of $F$. 

![Graphs of some Isotropic states](image-url)
Proof. From the graph structure of the state $\rho$, Eq. (37), we see that the family of subgraphs $\{\langle C_\mu, C_\nu \rangle\}$ do not satisfy the commutativity and normality criterion, except some specific edge weights.

As an example consider the subgraph $\langle C_1, C_2 \rangle$ of the graph $\rho_{3,x}$ depicted in the figure 4. The subgraph $\langle C_1, C_2 \rangle$ also breaks the normality condition for all non-zero edge weights due to reasons similar to those stated in the theorem 2.

Thus, we may conclude that graph Laplacian isotropic states have non-zero quantum discord except for some specific values of $F$. \hfill \square

5.3 X state

The X-state is well known in quantum information theory due to the specific structure of its density matrix. Discord of some classes of 2-qubit X-states have been studied in the literature [25, 26]. Here, we consider graph Laplacian (definition 1) X-states acting on $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$. Hence, as before the vertex set of the corresponding digraph has $m$ clusters $C_\mu, \mu = 1, 2, \ldots m$, each containing $n$ vertices. The distribution of the non-zero elements in the density matrices suggest that the edge set has the following combinatorial characteristics:

1. If the bipartite subgraph $\langle C_\mu, C_\nu \rangle$ is non-empty then all the edges are of the form $(v_{\mu k}, v_{\nu(n-k)})$ for $k = 1, 2, \ldots n$.

2. There is only one non-empty subgraph $\langle C_\alpha \rangle$ with edges of the form $(v_{\alpha k}, v_{\alpha(n-k)})$ for $k = 1, 2, \ldots n$.

Conversely if the edge set of any graph follows the above two properties the corresponding quantum states will be classified as an X state.

Example 4. Some of the graphs of X states without edge weights and directions are depicted in the figures 5a and 5b.

Theorem 4. A graph Laplacian X state acting on $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$ has zero quantum discord if and only if the following conditions are satisfied:

1. Any two non-empty subdigraphs of the form $\langle C_\mu, C_\nu \rangle$ are equal.

2. Degree of the vertices of $C_\mu$ will fulfill $d_\mu = d_{\mu(n-i)}$ for $i = 1, 2, \ldots n$.

Proof. Recall that if two subdigraphs $\langle C_\mu, C_\nu \rangle$ and $\langle C_\alpha, C_\beta \rangle$ are equal, then the commutativity condition is satisfied. Also, if any one of them is empty, the commutativity condition is again satisfied. Now we consider the subgraphs
\langle C_{\mu}, C_{\nu} \rangle \) and \( \langle C_{\alpha} \rangle \). When any one of them is an empty graph the commutativity condition is satisfied trivially. There is only one non-empty subgraph of the form \( \langle C_{\alpha} \rangle \). Using corollary 1 we may verify that the non-empty graphs \( \langle C_{\mu}, C_{\nu} \rangle \) and \( \langle C_{\alpha} \rangle \) are commutative. Also using lemma 3 we can show that subgraphs \( \langle C_{\mu}, C_{\nu} \rangle \) and \( \langle C_{\alpha} \rangle \) satisfy the conditions for being normal. Last, we shall check the degree condition,

\[ w(v_{\mu i}, v_{\nu j})(d_{\alpha i} - d_{\alpha j}) = 0. \] (39)

As \( \langle C_{\mu}, C_{\nu} \rangle \) is non-empty, we have \( w(v_{\mu i}, v_{\mu (n-i)}) \neq 0 \) for some \( i = 1, 2, \ldots n \). For those specific values of \( i \) we have,

\[ w(v_{\mu i}, v_{\nu (n-i)})(d_{\alpha i} - d_{\alpha (n-i)}) = 0. \] (40)

As \( w(v_{\mu i}, v_{\nu (n-i)}) \neq 0 \), we have \( d_{\alpha i} = d_{\alpha (n-i)} \) for \( i = 1, 2, \ldots n \).

6 Conclusions

This work extends our earlier work on quantum discord of graph Laplacian states arising from simple graphs to the graph Laplacian states arising from weighted digraphs that cover a wider set of quantum states represented by graphs. We establish that a quantum state \( \rho = \rho_{ij} \) is a graph Laplacian state if and only if \( \rho_{ij} \geq \sum_{i \neq j} \rho_{ij} \), that is, a diagonally dominant quantum state. For these density matrices we have constructed combinatorial criterion for zero quantum discord. Using this we proved that all the Werner states have nonzero quantum discord. Also an \( X \) state has zero discord if and only if the underlined graph follows a particular degree sequence.

We have shown that all Isotropic states are not graph Laplacian states and hence it would be worthwhile to develop graph theoretic representation of these states. This would help in the investigation of properties of a bigger class of quantum states with a corresponding pictorial description.
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References

[1] Samuel L Braunstein, Sibasish Ghosh, and Simone Severini. The laplacian of a graph as a density matrix: a basic combinatorial approach to separability of mixed states. *Annals of Combinatorics*, 10(3):291–317, 2006.

[2] Ali Hassan, M Saif, and Pramod S Joag. A combinatorial approach to multipartite quantum systems: basic formulation. *Journal of Physics A: Mathematical and Theoretical*, 40(33):10251, 2007.

[3] Supriyo Dutta, Bibhas Adhikari, and Subhashish Banerjee. A graph theoretical approach to states and unitary operations. *Quantum Information Processing*, 15(5):2193–2212, 2016.

[4] Joshua Lockhart and Simone Severini. Combinatorial entanglement. *arXiv preprint arXiv:1605.03564*, 2016.

[5] Abdelilah Belhaj, Adil Belhaj, Larbi Machkouri, Moulay Brahim Sedra, and Soumia Ziti. Weighted graph theory representation of quantum information inspired by lie algebras. *arXiv preprint arXiv:1609.03534*, 2016.

[6] David E Simmons, Justin P Coon, and Animesh Datta. Symmetric laplacians, quantum density matrices and their von-neumann entropy. *arXiv preprint arXiv:1703.01142*, 2017.

[7] Bibhas Adhikari, Subhashish Banerjee, Satyabrata Adhikari, and Atul Kumar. Laplacian matrices of weighted digraphs represented as quantum states. *Quantum information processing*, 16(3):79, 2017. arXiv: 1205.2747.

[8] Supriyo Dutta, Bibhas Adhikari, and Subhashish Banerjee. Quantum discord of states arising from graphs. *arXiv preprint arXiv:1702.06360*, 2017.

[9] Wojciech H Zurek. Einselection and decoherence from an information theory perspective. *arXiv preprint quant-ph/0011039*, 2000.

[10] Harold Ollivier and Wojciech H Zurek. Quantum discord: a measure of the quantumness of correlations. *Physical review letters*, 88(1):017901, 2001.

[11] Leah Henderson and Vlatko Vedral. Classical, quantum and total correlations. *Journal of physics A: mathematical and general*, 34(35):6899, 2001.
[12] Satyabrata Adhikari and Subhashish Banerjee. Operational meaning of discord in terms of teleportation fidelity. *Physical Review A*, 86(6):062313, 2012.

[13] Stefano Pirandola. Quantum discord as a resource for quantum cryptography. *arXiv preprint arXiv:1309.2446*, 2013.

[14] Aharon Brodutch and Daniel R Terno. Why should we care about quantum discord? *arXiv preprint arXiv:1608.01920*, 2016.

[15] Yichen Huang. Computing quantum discord is np-complete. *New Journal of Physics*, 16(3):033027, 2014.

[16] Jie-Hui Huang, Lei Wang, and Shi-Yao Zhu. A new criterion for zero quantum discord. *New Journal of Physics*, 13(6):063045, 2011.

[17] Borivoje Dakić, Vlatko Vedral, and Časlav Brukner. Necessary and sufficient condition for nonzero quantum discord. *Physical review letters*, 105(19):190502, 2010.

[18] Supriyo Dutta, Bibhas Adhikari, Subhashish Banerjee, and R Srikanth. Bipartite separability and nonlocal quantum operations on graphs. *Physical Review A*, 94(1):012306, 2016.

[19] Douglas Brent West. *Introduction to graph theory*, volume 2. Prentice hall Upper Saddle River, 2001.

[20] Marek Küs and Ingemar Bengtsson. classical quantum states. *Physical Review A*, 80(2):022319, 2009.

[21] Reinhard F Werner. Quantum states with einstein-podolsky-rosen correlations admitting a hidden-variable model. *Physical Review A*, 40(8):4277, 1989.

[22] Shunlong Luo. Using measurement-induced disturbance to characterize correlations as classical or quantum. *Physical Review A*, 77(2):022301, 2008.

[23] Shunlong Luo and Shuangshuang Fu. Geometric measure of quantum discord. *Physical Review A*, 82(3):034302, 2010.

[24] Yu Guo. Non-commutativity measure of quantum discord. *Scientific reports*, 6, 2016.

[25] Mazhar Ali, ARP Rau, and Gernot Alber. Quantum discord for two-qubit states. *Physical Review A*, 81(4):042105, 2010.

[26] Krishna Kumar Sabapathy and R Simon. Quantum discord for two-qubit states: A comprehensive approach inspired by classical polarization optics. *arXiv preprint arXiv:1311.0210*, 2013.