5

Graph Theoretic Aspects of Quantum Discord

Quantum discord [Henderson and Vedral, 2001; Ollivier and Zurek, 2001] $D(\rho)$ is a class of quantum correlations in quantum information [Brodutch and Terno, 2016; Pirandola, 2013]. The computation of discord involves optimization, making it a computationally challenging task. In fact, calculating quantum discord is an NP complete problem [Huang, 2014; Lim and Joynt, 2014]. Hence, the need to have an alternative formulation of quantum discord. In this chapter, we construct graph theoretical criterion of zero and non-zero quantum discord in graph Laplacian quantum states related to simple and weighted digraphs. Zero discord quantum states are known as classical quantum states or pointer states [Kuś and Bengtsson, 2009; Henderson and Vedral, 2001]. Correspondingly, it will be seen here that there are graph Laplacian pointer states. This chapter follows our two articles [Dutta et al., 2017a,b]. We begin this chapter with an introduction to the formulation of quantum discord. Then we shall find out some graphical conditions for constructing a family of normal commuting matrices. We use these criterion for constructing quantum states with zero and non-zero discord.

5.1 AN INTRODUCTION TO QUANTUM DISCORD

We begin by recapitulating a number of basic ideas in classical information theory [Cover and Thomas, 2012]. An elementary information source is a pair (X, p) where X is a finite set which is formally called an alphabet and p is a probability distribution on X that is $p : X \to [0, 1]$ is a map satisfying $\sum_{x \in X} p(x) = 1$. The quantity,

$$H(x) = -\sum_{x \in X} p(x) \log p(x) \tag{5.1}$$

is called the Shanon entropy [Shannon and Weaver, 1998] of the elementary information source (X, p), or simply the Shanon entropy of the probability distribution p. Here, X is a random variable whose probability distribution is p. The Shanon entropy has a crucial significance in information and coding theory [Parthasarathy, 2013]. It is a measure of information that is the uncertainty of a random variable.

Now we consider a joint probability distribution of two random variables X and Y, that is $((X, Y), p(x, y))$. The joint entropy is given by,

$$H(x, y) = -\sum_{x \in X} \sum_{y \in Y} p(x, y) \log p(x, y). \tag{5.2}$$

The conditional random variable is denoted by $Y|X$. The conditional entropy is given by

$$H(Y|X) = \sum_{x \in X} p(x) H(Y|X = x) = -\sum_{x \in X} \sum_{y \in Y} p(x, y) \log p(y|x). \tag{5.3}$$

Here $p(x)$ is the marginal probability distribution of the random variable X. The chain rule establishes a connection between joint entropy and conditional entropy which is given by,

$$H(X, Y) = H(X) + H(Y|X). \tag{5.4}$$

The relative entropy is a measure of distance between two probability distributions. The relative entropy between two probability mass functions $p(x)$ and $q(x)$ is defined by,

$$D(p||q) = \sum_{x \in X} p(x) \log \left(\frac{p(x)}{q(x)} \right). \tag{5.5}$$

It leads us to the definition of mutual information of two random variables X and Y which is denoted by $I(X;Y)$. Consider two random variables X and Y with the joint probability distribution $p(x, y)$ and marginal probability distributions $p(x)$ and $p(y)$. Now the mutual information is the relative entropy between the joint distribution $p(x, y)$ and the product distribution $p(x)p(y)$. Hence,

$$I(X;Y) = -\sum_{x \in X} \sum_{y \in Y} p(x, y) \log \left(\frac{p(x, y)}{p(x)p(y)} \right). \tag{5.6}$$

It can also be shown that

$$I(X;Y) = H(X) - H(X|Y). \tag{5.7}$$

Also applying the chain rule,

$$I(X;Y) = H(X) + H(Y) - H(X, Y). \tag{5.8}$$

In classical information theory the two equations provide equal quantitative values of $I(X;Y)$ but are different in quantum information theory.

In quantum information von-Neumann entropy is analogous to Shanon entropy. Given a density matrix ρ the von-Neumann entropy is defined by,

$$S(\rho) = \text{trace}(\rho \log(\rho)) = -\sum_i \lambda_i \log(\lambda_i), \tag{5.9}$$

where λ_i is an eigenvalues of the matrix ρ. Also, we assume that $0 \log(0) = 0$.

Let A and B are quantum systems with the corresponding Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. Let ρ be a bipartite density matrix in the combined Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. The reduced density matrices corresponding to the individual subsystems are

$$\rho_A = \text{trace}_B(\rho) \text{ and } \rho_B = \text{trace}_A(\rho), \tag{5.10}$$

where trace_A and trace_B are partial trace on the subsystems A and B.

Now from the equation (5.8) we can derive an expression of the quantum mutual information, which is

$$I(\rho) = S(\rho_A) + S(\rho_B) - S(\rho). \tag{5.11}$$

But the quantum mechanical analogue of (5.8) is not so straightforward.

Let $\{\Pi_i^B : i = 1, 2, \dots \dim(\mathcal{H}_B)\}$ be complete set of measurement operators corresponding to a von-Neumann measurement on the subsystem B. Let p_i be the probability for obtaining the outcome of the measurement Π_i^B that is

$$p_i = \text{trace}[(I_a \otimes \Pi_i^B)\rho(I_a \otimes \Pi_i^B)]. \tag{5.12}$$

The post measurement state of the system A is given by,

$$\rho_i^A = \frac{1}{p_i}\,\text{trace}_B\left((I_a \otimes \Pi_i^B)\rho(I_a \otimes \Pi_i^B)\right). \tag{5.13}$$

It was shown in [Ollivier and Zurek, 2001] that with respect to the measure $\{\Pi^B\}$ the conditional entropy of system A is

$$S(A|\{\Pi_i^B\}) = \sum_i p_i S(\rho_i^A). \tag{5.14}$$

The quantum mechanical analogue of equation (5.7) with respect to the measurement $\{\Pi_i^B\}$ is given by,

$$I(\rho|\Pi^B) = S(\rho_A) - S(A|\{\Pi_i^B\}). \tag{5.15}$$

The quantum discord [Henderson and Vedral, 2001; Ollivier and Zurek, 2001] is the quantum mechanical difference between two classically equivalent definitions of mutual information.

Definition 5.1. Quantum discord: *The quantum discord of a bipartite state ρ is*

$$D(\rho) = \min_{\Pi^B}\{I(\rho) - I(\rho|\Pi^B)\}. \tag{5.16}$$

In quantum information, quantum discord is a measure of non-classical correlations between two systems A and B, different from entanglement. Thus, there are separable quantum states with non-zero discord. Also all entangled states has non-zero discord. There are quantum states for which $D(\rho) = 0$. We call them classical-quantum states [Kuś and Bengtsson, 2009] or pointer states. From the perspective of computational complexity, it has been proved that calculating $D(\rho)$ is an NP-complete problem [Huang, 2014]. 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 developed in [Huang et al., 2011; Dakić et al., 2010].

Recall from equation (2.17) that, if we consider the canonical computational basis $\{|i_a\rangle\}$ of $\mathcal{H}_A$, and $\{|i_b\rangle\}$ of $\mathcal{H}_B$, then we can express ρ as,

$$\rho = \sum_{i,j} E_{ij} \otimes B_{ij}, \tag{5.17}$$

where, $E_{ij} = |i_a\rangle\langle j_a|$, and $B_{i,j} = \text{trace}_a[(|j_a\rangle\langle i_a| \otimes I_b)\rho]$. Therefore, B_{ij} are blocks of the density matrix ρ. It is proved in [Huang et al., 2011] that a quantum state represented by a density matrix ρ has zero discord if and only if $\{B_{ij}\}$ is a family of commuting normal matrices. Recall that two matrices A and B commute if $AB = BA$ holds. Also a matrix A is a normal matrix if it commutes with this conjugate transpose, that is $AA^\dagger = A^\dagger A$. A set of matrices $\{A_i : i = 1, 2, \dots\}$ is a family of commuting normal matrices if every A_i is a normal matrix and $A_iA_j = A_jA_i$ for all $i \neq j$. Properties of the family of commuting normal matrices are reviewed in [Horn and Johnson, 2012] and have applications in different branches of science and technology.

5.2 GRAPH THEORETIC ASPECTS OF COMMUTING NORMAL MATRICES

Recall that, a quantum state in $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$ is represented by a density matrix ρ of order $mn \times mn$ which is a block matrix with each block of size n. In subsection 2.2.6, we have partitioned the graph into clusters which is given by

$$\begin{aligned} &V = C_1 \cup C_2 \cup \dots \cup C_m;\\ &C_\mu \cap C_\nu = \emptyset \text{ for } \mu \neq \nu \text{ and } \mu, \nu = 1, 2, \dots m;\\ &C_\mu = \{v_{\mu 1}, v_{\mu 2}, \dots v_{\mu n}\}. \end{aligned} \tag{5.18}$$

It leads the adjacency matrix to be partitioned into block matrix as $A(G) = (A_{\mu\nu})$. Similarly, the block matrix representation of density matrix is given by $\rho(G) = (B_{\mu\nu})$. The relation between $(A_{\mu\nu})$ and $(B_{\mu\nu})$ is given in the equation (2.18) and is as detailed below.

$$B_{\mu\nu} = \begin{cases} s\frac{A_{\mu\nu}}{d} & \text{if } \mu \neq \nu \\ \frac{D_\mu + sA_{\mu\mu}}{d} & \text{if } \mu = \nu, \end{cases} \tag{5.19}$$

where $s = 1$ for $\rho_q(G)$ and $s = -1$ for $\rho_l(G)$. Also, we have discussed the relationship between blocks of the adjacency matrix and the subgraphs generated by these clusters, in the subsection 2.2.6. We require all these relationships for further investigations in this chapter and the next one. Note that, the commuting normality property of blocks of the graph Laplacian states are determined by the structural properties of $\langle C_\mu \rangle$ and $\langle C_\mu, C_\nu \rangle$. We break this section into two parts: one for simple graphs, and another for weighted digraphs.

5.2.1 Commuting normal matrices generated by the blocks of simple graphs

We have assumed graph Laplacian quantum states related to the simple graphs in this section. We investigate a number of structural properties on the subgraphs $\langle C_\mu \rangle$, and $\langle C_\mu, C_\nu \rangle$, such that, $B_{\mu,\nu}$ are normal and commutating. Note that, $A_{\mu,\nu}$ are binary matrices as the underlined graph is a simple graph.

Definition 5.2. Support of a vector: *Given any binary vector a, we define, the support of a as,*

$$\text{nbd}(a) = \{i(\text{mod } n) : a(i) = 1\}. \tag{5.20}$$

In the above definition $i(\text{mod } n)$ will be calculated with usual modular arithmetic. Also, n will be chosen from the context. Let a, and b be two binary vectors. The product,

$$(a, b) = \#(\text{nbd}(a) \cap \text{nbd}(b)). \tag{5.21}$$

For a binary matrix $A = (a_{ij})_{n\times n}$, we denote a_{i*} and a_{*j} as i-th row and j-th column vector, respectively. Corresponding to every A, there is a simple bipartite graph of order $2n$, $\mathcal{A} = (V(\mathcal{A}), E(\mathcal{A}))$ with adjacency matrix,

$$A(\mathcal{A}) = \begin{bmatrix} 0 & A \\ A^\dagger & 0 \end{bmatrix}. \tag{5.22}$$

Let bipartitions of $V(\mathcal{A})$ are C_μ and C_ν, where $C_\mu = \{v_{\mu,1}, v_{\mu,2}, \dots v_{\mu,n}\}$, $C_\nu = \{v_{\nu,1}, v_{\nu,2}, \dots v_{\nu,n}\}$. Recall that, given any vertex $v_{\gamma i}$, the index i represents the position of a vertex in γ-th cluster, where $\gamma = \mu, \nu$, etc. An undirected edge $(v_{\mu i}, v_{\nu j}) \in E(\mathcal{A})$, if and only if $a_{ij} = 1$. Thus, $\mathcal{A} = \langle C_\mu, C_\nu \rangle$. As $\mathcal{A}$ is bipartite, the neighbourhood of a vertex $v_{\mu i}$ in $\mathcal{A}$ is a subset of C_ν,

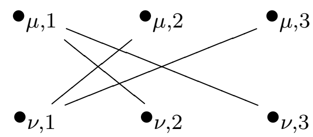
$$\text{Nbd}_{\mathcal{A}}(v_{\mu i}) = \{v_{\nu j} : (v_{\mu i}, v_{\nu j}) \in E(G)\}. \tag{5.23}$$

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 $(0_{1,n}, a_{i*})$ represents edges incident to $v_{\mu i}$. Thus, $\text{nbd}(0_{1,n}, a_{i*}) = \text{nbd}(a_{i*})$ represents indexes of vertices in $\text{Nbd}_{\mathcal{A}}(v_{\mu i})$. Hence, we write $\text{nbd}(a_{i*})$ as $\text{nbd}_{\mathcal{A}}(v_{\mu i})$. Similarly, the $(n + i)$-th column of $A(\mathcal{A})$, that is $(a_{*i}, 0_{n,1})$ represents edges incident to $v_{\nu i}$. $\text{nbd}(0_{n,1}, a_{*i}) = \text{nbd}(a_{*i})$ represents indexes of vertices in $\text{Nbd}_{\mathcal{A}}(v_{\nu i})$. We also denote the set $\text{nbd}(a_{*i})$ as $\text{nbd}_{\mathcal{A}}(v_{\nu i})$. Precisely, we may combine the above text as,

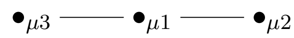
$$\begin{aligned} \text{nbd}_{\mathcal{A}}(v_{\mu i}) &= \{j : v_{\nu j} \in \text{Nbd}_{\mathcal{A}}(v_{\mu j})\} = \text{nbd}(a_{i*}), \\ \text{and } \text{nbd}_{\mathcal{A}}(v_{\nu i}) &= \{j : v_{\mu j} \in \text{Nbd}_{\mathcal{A}}(v_{\nu j})\} = \text{nbd}(a_{*i}). \end{aligned} \tag{5.24}$$

In particular, any binary symmetric matrix A of order n with zero diagonal entries may be considered as an adjacency matrix of a graph $\overline{A}$. Let $V(\overline{A}) = C_\mu = \{v_{\mu,1}, v_{\mu,2}, \dots v_{\mu,n}\}$. The edge $(v_{\mu,i}, v_{\mu,j}) \in E(\overline{A})$ if and only if $a_{ij} \neq 0$. Thus, $\overline{A} = \langle C_\mu \rangle$.

Example 5.1. *Consider the matrix* $A = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$. *Corresponding bipartite graph, $\mathcal{A}$, is as follows.*



Consider, $a_{*1} = (0, 1, 1)^\dagger$, *that is* $\mathrm{nbd}(a_{*1}) = \{2, 3\}$. *Note that,* $\mathrm{Nbd}_{\mathcal{A}}(v_{\nu 1}) = \{v_{\mu,2}, v_{\mu,3}\}$. *Also, A is a symmetric binary matrix with zero diagonal entries. Thus, A is the adjacency matrix of a graph $\overline{A}$, depicted below,*



Lemma 5.1. *Let bipartite graphs corresponding to binary matrices A, and B of order n be $\mathcal{A} = \langle C_\mu, C_\nu \rangle$, and $\mathcal{B} = \langle C_\alpha, C_\beta \rangle$, respectively. They commute, if and only if for all i, j with $1 \leq i, j \leq n$,*

$$\#(\mathrm{nbd}(v_{\mu i}) \cap \mathrm{nbd}(v_{\beta j})) = \#(\mathrm{nbd}(v_{\nu j}) \cap \mathrm{nbd}(v_{\alpha i})).$$

Proof. For commutativity $AB = BA$ holds if and only if $(AB)_{ij} = (BA)_{ij}$ for all i, j with $1 \leq i, j \leq n$. Now applying equation (5.21) we get,

$$\begin{aligned} (AB)_{ij} &= \sum_{k=1}^{n} a_{ik} b_{kj} = \langle a_{i*}, b_{*j} \rangle = \#(\mathrm{nbd}(v_{\mu i}) \cap \mathrm{nbd}(v_{\beta j})), \\ (BA)_{ij} &= \sum_{k=1}^{n} b_{ik} a_{kj} = \langle b_{i*}, a_{*j} \rangle = \#(\mathrm{nbd}(v_{\nu j}) \cap \mathrm{nbd}(v_{\alpha i})). \end{aligned} \tag{5.25}$$

□

When A, and B do not commute, the above lemma does not hold. Thus, the non-commutativity of A and B is reflected in the edge sets of the graphs $\mathcal{A}$, and $\mathcal{B}$. We can assume the following quantity as a measure of non-commutativity of A and B,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \left| \#(\mathrm{nbd}(v_{\mu i}) \cap \mathrm{nbd}(v_{\beta j})) - \#(\mathrm{nbd}(v_{\nu j}) \cap \mathrm{nbd}(v_{\alpha i})) \right|. \tag{5.26}$$

Corollary 5.1. *Let $\overline{A} = \langle C_\mu \rangle$, and $\mathcal{B} = \langle C_\alpha, C_\beta \rangle$ be graphs corresponding to a binary symmetric matrix $A = (a_{ij})_{n \times n}$ with zero diagonal entries, and any binary matrix $B = (b_{ij})_{n \times n}$. They commute if and only if for all i, j with $1 \leq i, j \leq n$,*

$$\#(\mathrm{nbd}(v_{\mu i}) \cap \mathrm{nbd}(v_{\beta j})) = \#(\mathrm{nbd}(v_{\mu j}) \cap \mathrm{nbd}(v_{\alpha i})).$$

Proof. We have already justified that, $\mathrm{nbd}(a_{i*}) = \mathrm{nbd}(v_{\mu i}) = \mathrm{nbd}(a_{*i})$, for all $i = 1, 2, \dots n$. From equation (5.25) we get, A commutes with B, if and only if $\langle a_{i*}, b_{*j} \rangle = \langle b_{i*}, a_{*j} \rangle$ for all i, and j. Applying the symmetry of A, we get, $\langle a_{i*}, b_{*j} \rangle = \langle a_{j*}, b_{i*} \rangle$. Using the graph theoretic convention, we get $\#(\mathrm{nbd}(v_{\mu i}) \cap \mathrm{nbd}(v_{\beta j})) = \#(\mathrm{nbd}(v_{\mu j}) \cap \mathrm{nbd}(v_{\alpha i}))$. □

When A and B do not commute we may measure the non-commutativity with the following quantity:

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left|\#(\text{nbd}(v_{\mu i})\cap\text{nbd}(v_{\beta j}))-\#(\text{nbd}(v_{\mu j})\cap\text{nbd}(v_{\alpha i}))\right|. \tag{5.27}$$

Corollary 5.2. *Two binary symmetric matrices with zero diagonal entries $A=(a_{ij})_{n\times n}$, and $B=(b_{ij})_{n\times n}$ corresponding to graphs $\overline{A}=\langle C_\mu\rangle$, and $\overline{B}=\langle C_\nu\rangle$ commute, if and only if for every i,j with $1\leq i,j\leq n$,*

$$\#(\text{nbd}(v_{\mu i})\cap\text{nbd}(v_{\nu j}))=\#(\text{nbd}(v_{\mu j})\cap\text{nbd}(v_{\nu i})).$$

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

In a similar fashion, the non-commutativity of A and B can be measured with,

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left|\#(\text{nbd}(v_{\mu i})\cap\text{nbd}(v_{\nu j}))-\#(\text{nbd}(v_{\mu j})\cap\text{nbd}(v_{\nu i}))\right|. \tag{5.28}$$

A binary 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 5.2. *Let $\mathcal{A}=\langle C_\mu,C_\nu\rangle$ be a bipartite graph corresponding to a binary matrix $A=(a_{ij})_{n\times n}$. It is normal, if and only if for every i, and j with $1\leq i,j\leq n$,*

$$\#(\text{nbd}(v_{\mu i})\cap\text{nbd}(v_{\mu j}))=\#(\text{nbd}(v_{\nu i})\cap\text{nbd}(v_{\nu j})).$$

Proof. Let $B=(b_{ij})_{n\times n}=(a_{ji})_{n\times n}=A^\dagger$. Clearly, $b_{i*}=a_{*i}$ and $b_{*i}=a_{i*}$ for all i. Note that,

$$(AA^\dagger)_{ij}=\sum_{k=1}^{n}a_{ik}b_{kj}=\langle a_{i*},b_{*j}\rangle=\langle a_{i*},a_{j*}\rangle=\#(\text{nbd}(v_{\mu i})\cap\text{nbd}(v_{\mu j})). \tag{5.29}$$

Similarly, $(A^\dagger A)_{ij}=\#(\text{nbd}(v_{\nu i})\cap\text{nbd}(v_{\nu j}))$. Hence, for any two i, and j with $1\leq i,j\leq n$ we have, $\#(\text{nbd}(v_{\mu i})\cap\text{nbd}(v_{\mu j}))=\#(\text{nbd}(v_{\nu i})\cap\text{nbd}(v_{\nu j}))$. □

When A is not a normal matrix we may measure its non-normality in terms of the edges of $\mathcal{A}$. The following quantity may be accepted as a measure of non-normality,

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left|\#(\text{nbd}(v_{\mu i})\cap\text{nbd}(v_{\mu j}))-\#(\text{nbd}(v_{\nu i})\cap\text{nbd}(v_{\nu j}))\right|. \tag{5.30}$$

Example 5.2. *The zero matrix Θ_n, the identity matrices I_n and the all one matrix J_n are three binary symmetric normal matrices. They also commute with all other matrices. Graphs corresponding to Θ_n are empty graphs. The bipartite graph $\mathcal{I}$ corresponding to I is depicted in the figure 5.1. The bipartite graph $\mathcal{J}$ corresponding to J_n is a complete bipartite graph $K_{n,n}$. Graph $K_{3,3}$ is depicted in the figure 5.2a. Another important binary symmetric matrix is J_n-I_n. The graph $\overline{J_n-I_n}$ is a complete graph K_n.*

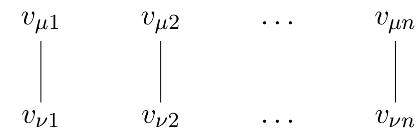


Figure 5.1 : Bipartite graph corresponding to the identity matrix I

5.2.2 Commuting normal matrices generated by the blocks of weighted digraphs

In this subsection, we find out conditions on a weighted digraph G such that the blocks of $\rho(G)$ form a family of normal commuting matrix. We consider only those weighted digraphs satisfying our basic assumptions 2.1.

Given a vertex i of a weighted digraph G we call the set $\text{nbd}_G(i) = \{j : j \in V(G), (i, j) \in E(G)\}$ as the neighbourhood of vertex i. According to our assumption (i, j) and (j, i) belong to $E(G)$ together. Thus, the neighbourhood determined by incoming edges, and out-going edges are equivalent. Due to its requirement in the next section we now develop the terminology of the neighbourhood.

For a labelled digraph G corresponding to any vertex i there is an ordered set of vertices, called an outer neighbourhood of i denoted and defined by,

$$\text{Nbd}_G(i)_{out} = \{j : j \in V(G), (i, j) \in E(G)\}. \tag{5.31}$$

Also we define,

$$\text{Nbd}_G(i)_{in} = \{j : j \in V(G), (j, i) \in E(G)\}. \tag{5.32}$$

Corresponding to the sets $\text{Nbd}_G(i)_{out}$ and $\text{Nbd}_G(i)_{in}$ there are multi-sets of edge weights denoted and defined by,

$$W(\text{Nbd}_G(i)_{out}) = \{w_G(i, j) : j \in \text{Nbd}_G(i)_{out}, (i, j) \in E(G)\}, \tag{5.33}$$

$$W(\text{Nbd}_G(i)_{in}) = \{w_G(j, i) : j \in \text{Nbd}_G(i)_{in}, (j, i) \in E(G)\}. \tag{5.34}$$

Given a vertex i we call the set $\text{nbd}_G(i) = \{j : j \in V(G), (i, j) \in E(G)\}$ as the neighbourhood 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:

$$\begin{aligned} W(\text{nbd}_G(i)_{out}) &= \{w_G(i, j) : (i, j) \in E(G)\}, \\ W(\text{nbd}_G(i)_{in}) &= \{w_G(j, i) : (j, i) \in E(G)\}. \end{aligned} \tag{5.35}$$

Definition 5.3. Support of a vector: *Given a vector $a \in \mathbb{C}^n$ there is a set of natural numbers* $\text{nbd}(a)$ *defined by,*

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

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

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

$$(a, b) = \sum_{k \in \text{nbd}(a) \cap \text{nbd}(b)} a(k)b(k). \tag{5.36}$$

Given a matrix $A = (a_{ij})_{n\times n}$, a_{i*} and a_{*j} denotes the i-th row and j-th column vectors, respectively. Corresponding to every A, there is a weighted bipartite graph of order $2n$, $\mathcal{A} = (V(\mathcal{A}), E(\mathcal{A}))$ with the adjacency matrix,

$$A(\mathcal{A}) = \begin{bmatrix} 0 & A \\ A^\dagger & 0 \end{bmatrix}. \tag{5.37}$$

As $\mathcal{A}$ is a bipartite graph we can write $V(\mathcal{A}) = C_\mu \cup C_\nu$, where $C_\mu = \{v_{\mu 1}, v_{\mu 2}, \dots v_{\mu n}\}$, $C_\nu = \{v_{\nu 1}, v_{\nu 2}, \dots v_{\nu n}\}$ and $C_\mu \cap C_\nu = \emptyset$ as mentioned in equation (2.14). Therefore, $\mathcal{A} = \langle C_\mu, C_\nu\rangle$, the subgraph generated by the vertex sets C_μ and C_ν. 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,

$$\text{nbd}_{\mathcal{A}}(v_{\mu i}) = \{v_{\nu j} : (v_{\mu i}, v_{\nu j}) \in E(G)\} \subset C_\nu. \tag{5.38}$$

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 $(0_{1,n}, a_{i*})$ represents weights of outgoing edges from the vertex $v_{\mu i}$. According to the definition 5.3, $\text{nbd}(0_{1,n}, a_{i*}) = \text{nbd}(a_{i*})$ which represents indexes of vertices in $\text{nbd}_{\mathcal{A}}(v_{\mu i})$. Thus we have,

$$\text{nbd}(a_{i*}) = \text{nbd}_{\mathcal{A}}(v_{\mu i}), \text{ and } a_{i*} = W(\text{nbd}_{\mathcal{A}}(v_{\mu i})_{out}). \tag{5.39}$$

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

$$\text{nbd}(a_{*i}) = \text{nbd}_{\mathcal{A}}(v_{\nu i}) \text{ and } a_{*i} = W(\text{nbd}_{\mathcal{A}}(v_{\nu i})_{in}). \tag{5.40}$$

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

Lemma 5.3. *Let the weighted bipartite digraphs corresponding to complex square matrices A and B of order n be $\mathcal{A} = \langle C_\mu, C_\nu\rangle$, and $\mathcal{B} = \langle C_\alpha, C_\beta\rangle$, respectively. The matrices A and B commute, if and only if for all i, j with $1 \leq i, j \leq n$,*

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

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 $b_{kj} = w(v_{\alpha k}, v_{\beta j})$. Now applying equation (5.36) we get,

$$\begin{aligned} (AB)_{ij} &= \sum_{k=1}^{n} a_{ik} b_{kj} = \langle a_{i*}, b_{*j}\rangle = \sum_{k} w(v_{\mu i}, v_{\nu k}) w(v_{\alpha k}, v_{\beta j}) : k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\beta j}), \\ (BA)_{ij} &= \sum_{k=1}^{n} b_{ik} a_{kj} = \langle b_{i*}, a_{*j}\rangle = \sum_{k} w(v_{\alpha i}, v_{\beta k}) w(v_{\mu k}, v_{\nu j}) : k \in \text{nbd}(v_{\alpha i}) \cap \text{nbd}(v_{\nu j}). \end{aligned} \tag{5.41}$$

□

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 5.3. *Let $\tilde{A} = \langle C_\mu \rangle$, and $\mathcal{B} = \langle C_\alpha, C_\beta \rangle$ be graphs corresponding to a Hermitian matrix $A = (a_{ij})_{n\times n}$, and square matrix $B = (b_{ij})_{n\times n}$. They commutes if and only if for all i, j with $1 \le i, j \le n$,*

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

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

Corollary 5.4. *Two Hermitian matrices $A = (a_{ij})_{n\times n}$, and $B = (b_{ij})_{n\times n}$ corresponding to graphs $\tilde{A} = \langle C_\mu \rangle$, and $\tilde{B} = \langle C_\nu \rangle$ commute, if and only if for every i, j with $1 \le i, j \le n$,*

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

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

Lemma 5.4. *Let $\mathcal{A} = \langle C_\mu, C_\nu \rangle$ 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, and j with $1 \le i, j \le n$,*

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

Proof. Let $B = (b_{ij})_{n\times n} = (a_{ji})_{n\times n} = A^\dagger$. Clearly, $b_{i*} = a^\dagger_{*i}$ and $b_{*i} = a^\dagger_{i*}$ for all i. Note that,

$$\begin{aligned}(AA^\dagger)_{ij} &= \sum_{k=1}^{n} a_{ik} b_{kj} = \langle a_{i*}, b_{*j}\rangle = \langle a_{i*}, a_{j*}\rangle \\ &= \sum_{k} w(v_{\mu i}, v_{\nu k}) w(v_{\nu k}, v_{\mu j}) : k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\mu j}).\end{aligned} \tag{5.42}$$

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. □

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_μ and C_ν. Now, for $i = j = p$,

$$\sum_{k\in \text{nbd}(v_{\mu i})\cap \text{nbd}(v_{\mu j})} w(v_{\mu i}, v_{\nu k}) w(v_{\nu k}, v_{\mu j}) = w(v_{\mu p}, v_{\nu q}) w(v_{\nu q}, v_{\mu p}). \tag{5.43}$$

Also, for $i = j = p$ the set $\text{nbd}(v_{\nu i}) \cap \text{nbd}(v_{\nu j}) = \emptyset$, as $v_{\nu p}$ is an isolated vertex. Hence, the term $\sum_{k\in \text{nbd}(v_{\nu i})\cap \text{nbd}(v_{\nu j})} w(v_{\nu i}, v_{\mu k}) w(v_{\mu k}, v_{\nu j})$ takes no value. In this case, the graph $\langle C_\mu, C_\nu \rangle$ fails to fulfil 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.

5.3 DISCORD OF GRAPH LAPLACIAN QUANTUM STATES IN GENERAL

In the last section, we have realized that blocks of a density matrix $\rho(G)$ forms a family of normal commuting matrices depending on the structure of the graph G. In graph theoretic terms, a graph Laplacian quantum state $\rho(G)$ has zero quantum discord if these followings properties of block matrices are satisfied.

1. Normality of $B_{\mu\mu}$, that is of $D_\mu \pm A_{\mu\mu}$ for all μ.
2. Normality of $B_{\mu\nu}$, that is of $A_{\mu\nu}$ for all $\mu \neq \nu$.
3. Commutativity of $B_{\mu\nu}$, and $B_{\alpha\beta}$, that is between $A_{\mu\nu}$, and $A_{\alpha\beta}$, where $\mu \neq \nu$, and $\alpha \neq \beta$.
4. Commutativity between $B_{\mu\mu}$, and $B_{\alpha\beta}$, that is $D_\mu \pm A_{\mu\mu}$, and $A_{\alpha\beta}$, where $\alpha \neq \beta$.
5. Commutativity between $B_{\mu\mu}$, and $B_{\nu\nu}$, that is between $D_\mu \pm A_{\mu\mu}$, and $D_\nu \pm A_{\nu\nu}$.

In this section, we shall discuss about discord in graph Laplacian quantum states based on the above properties. We shall find out simple and weighted digraphs such that the corresponding quantum states has zero discord. Also, we shall provide a graph theoretic measure of quantum discord for simple graphs.

5.3.1 Zero discord graph Laplacian states related to simple graphs

The Property 1 holds trivially for all graphs because symmetric matrices are normal. The matrix $A_{\mu\mu}$, and D_μ are adjacency matrix, and degree matrix, respectively of the induced subgraph $\langle C_\mu \rangle$. They are symmetric. Thus, $B_{\mu\mu} = D_\mu \pm A_{\mu\mu}$ are normal matrices for all μ.

The Property 2 is satisfied by all those graphs for which all the subgraphs $\langle C_\mu, C_\nu \rangle$ meet the normality condition in Lemma 5.2. If there are some block matrices $B_{\mu\nu}$, which are not normal, we may measure the violation of normality by the graph G using the following sum,

$$P = \sum_{\mu=1}^{m} \sum_{\nu=1}^{m} \sum_{i=1}^{n} \sum_{j=1}^{n} \left| \#(\text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\mu j})) - \#(\text{nbd}(v_{\nu i}) \cap \text{nbd}(v_{\nu j})) \right|. \tag{5.44}$$

It comes from the equation (5.30) after adding on all possible subgraphs $\langle C_\mu, C_\nu \rangle$ of G.

The Property 3 is satisfied by all those graphs for which any two subgraphs $\langle C_\mu, C_\nu \rangle$, and $\langle C_\alpha, C_\beta \rangle$ fulfil the lemma (5.1). If any two blocks do not commute, we may measure the existing non-commutativity in the graph using the equation (5.26) with the following quantity,

$$Q = \sum_{\mu=1}^{m} \sum_{\nu=1}^{m} \sum_{i=1}^{n} \sum_{j=1}^{n} \left| \#(\text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\beta j})) - \#(\text{nbd}(v_{\nu j}) \cap \text{nbd}(v_{\alpha i})) \right|. \tag{5.45}$$

The property 4 deals with commutativity between $B_{\mu\mu}$ and $B_{\alpha\beta}$, that is the graph will satisfy $B_{\mu\mu} B_{\alpha\beta} = B_{\alpha\beta} B_{\mu\mu}$ for all μ, α, and β. It indicates,

$$\begin{aligned} &\frac{1}{d}(D_\mu \pm A_{\mu\mu}) \frac{\pm 1}{d} A_{\alpha\beta} = \frac{\pm 1}{d} A_{\alpha\beta} \frac{1}{d}(D_\mu \pm A_{\mu\mu}) \\ &\text{or } D_\mu A_{\alpha\beta} \pm A_{\mu\mu} A_{\alpha\beta} = A_{\alpha\beta} D_\mu \pm A_{\alpha\beta} A_{\mu\mu}. \end{aligned} \tag{5.46}$$

Rearranging its terms we get the equation,

$$(D_\mu A_{\alpha\beta} - A_{\alpha\beta} D_\mu) \pm (A_{\mu\mu} A_{\alpha\beta} - A_{\alpha\beta} A_{\mu\mu}) = 0. \tag{5.47}$$

Note that, D_μ, and $A_{\mu\mu}$ are degree, and adjacency matrices of $\langle C_\mu \rangle$, respectively. Also, $A_{\alpha\beta}$ corresponds the bipartite graph $\langle C_\alpha, C_\beta \rangle$. The above equation holds if for all i, j with $1 \le i, j \le n$,

$$\begin{aligned} &(D_\mu A_{\alpha\beta})_{ij} - (A_{\alpha\beta} D_\mu)_{ij} \pm \{(A_{\mu\mu} A_{\alpha\beta})_{ij} - (A_{\alpha\beta} A_{\mu\mu})_{ij}\} = 0 \\ \text{or } &d_{\mu i}(A_{\alpha\beta})_{ij} - (A_{\alpha\beta})_{ij} d_{\mu j} \pm \{(A_{\mu\mu} A_{\alpha\beta})_{ij} - (A_{\alpha\beta} A_{\mu\mu})_{ij}\} = 0. \end{aligned} \tag{5.48}$$

Now, $(A_{\alpha\beta})_{ij}$ is either zero or one depending on existence of the edge $(v_{\alpha i}, v_{\beta j})$. Commutativity of $A_{\mu\mu}$ and $A_{\alpha\beta}$ has been discussed in the Corollary 5.1. Applying it in the above equation we get,

$$\mathcal{X}_{\alpha\beta}(i,j)(d_{\mu i} - d_{\mu j}) \pm \left[\#(\text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\beta j})) - \#(\text{nbd}(v_{\mu j}) \cap \text{nbd}(v_{\alpha i}))\right] = 0. \tag{5.49}$$

Observe that, if vertices of $C_\mu, \mu = 1, 2, \dots m$ 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 5.1. Violation of the Property 4 can be measured by,

$$R = \sum_{\mu=1}^{m} \sum_{\nu=1}^{m} \sum_{i=1}^{n} \sum_{j=1}^{n} \left| \mathcal{X}_{\alpha\beta}(i,j)(d_{\mu i} - d_{\mu j}) \pm \left[\#(\text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\beta j})) - \#(\text{nbd}(v_{\mu j}) \cap \text{nbd}(v_{\alpha i}))\right] \right|. \tag{5.50}$$

We consider '$+$' sign for $\rho_q(G)$ and '$-$' sign for $\rho_l(G)$ in the above expression.

The Property 5 requires commutativity of $B_{\mu\mu}$ and $B_{\nu\nu}$, that is $B_{\mu\mu} B_{\nu\nu} = B_{\nu\nu} B_{\mu\mu}$. It indicates,

$$\begin{aligned} &\frac{1}{d}(D_\mu \pm A_{\mu\mu}) \frac{1}{d}(D_\nu \pm A_{\nu\nu}) = \frac{1}{d}(D_\nu \pm A_{\nu\nu}) \frac{1}{d}(D_\mu \pm A_{\mu\mu}) \\ \text{or } &D_\mu D_\nu \pm D_\mu A_{\nu\nu} \pm A_{\mu\mu} D_\nu + A_{\mu\mu} A_{\nu\nu} = D_\nu D_\mu \pm D_\nu A_{\mu\mu} \pm A_{\nu\nu} D_\mu + A_{\nu\nu} A_{\mu\mu} \\ \text{or } &(A_{\mu\mu} A_{\nu\nu} - A_{\nu\nu} A_{\mu\mu}) \pm (D_\mu A_{\nu\nu} - A_{\nu\nu} D_\mu) \pm (A_{\mu\mu} D_\nu - D_\nu A_{\mu\mu}) = 0 \\ \text{or } &(A_{\mu\mu} A_{\nu\nu} - A_{\nu\nu} A_{\mu\mu})_{ij} \pm (D_\mu A_{\nu\nu} - A_{\nu\nu} D_\mu)_{ij} \pm (A_{\mu\mu} D_\nu - D_\nu A_{\mu\mu})_{ij} = 0, \end{aligned} \tag{5.51}$$

holds for all i, j with $1 \le i, j \le n$. Commutativity of $A_{\mu\mu}$, and $A_{\nu\nu}$ is discussed in the Corollary 5.2. We may write,

$$(A_{\mu\mu} A_{\nu\nu} - A_{\nu\nu} A_{\mu\mu})_{ij} = \#(\text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})) - \#(\text{nbd}(v_{\mu j}) \cap \text{nbd}(v_{\nu i})). \tag{5.52}$$

Also,

$$(D_\mu A_{\nu\nu} - A_{\nu\nu} D_\mu)_{ij} = d_{\mu i}(A_{\nu\nu})_{ij} - (A_{\nu\nu})_{ij} d_{\mu j} = \mathcal{X}_{\nu\nu}(i,j)(d_{\mu i} - d_{\mu j}) \tag{5.53}$$

$$(A_{\mu\mu} D_\nu - D_\nu A_{\mu\mu})_{ij} = (A_{\mu\mu})_{ij} d_{\nu j} - d_{\nu i}(A_{\nu\nu})_{ij} = \mathcal{X}_{\mu\mu}(i,j)(d_{\nu j} - d_{\nu i}). \tag{5.54}$$

Combining them together, we get

$$\begin{aligned} \left[\#(\text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})) - \#(\text{nbd}(v_{\mu j}) \cap \text{nbd}(v_{\nu i}))\right] &\pm \left[\mathcal{X}_{\nu\nu}(i,j)(d_{\mu i} - d_{\mu j})\right] \\ &\pm \left[\mathcal{X}_{\mu\mu}(i,j)(d_{\nu j} - d_{\nu i})\right] = 0. \end{aligned} \tag{5.55}$$

Note that, if vertices of $C_\mu, \mu = 1, 2, \dots m$ have equal degree, then $d_{\mu i} - d_{\mu j} = 0$ as well as $d_{\nu j} - d_{\nu i} = 0$. Then, G satisfies the Property 5, if and only if for any two subgraphs $\langle C_\mu \rangle$ and $\langle C_\nu \rangle$, conditions of Corollary 5.2 is fulfilled. We may measure violation of the Property 5 by the quantity,

$$\begin{aligned} S = \sum_{\mu=1}^{m} \sum_{\nu=1}^{m} \sum_{i=1}^{n} \sum_{j=1}^{n} \Big| &\left[\#(\text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})) - \#(\text{nbd}(v_{\mu j}) \cap \text{nbd}(v_{\nu i}))\right] \\ &\pm \left[\mathcal{X}_{\nu\nu}(i,j)(d_{\mu i} - d_{\mu j})\right] \pm \left[\mathcal{X}_{\mu\mu}(i,j)(d_{\nu j} - d_{\nu i})\right] \Big|. \end{aligned} \tag{5.56}$$

Here, '+' sign will be used for $\rho_q(G)$ and '−' sign will be used for $\rho_l(G)$.

Finding out all graphs satisfying all five structural properties is difficult. Here, we state a number of sufficient conditions on graphs representing zero discord quantum states.

Theorem 5.1. *Let the graph G have the following structural properties:*

1. *Degrees of the vertices in a cluster C_μ is equal for all $\mu = 1, 2, \dots m$.*
2. *Any pair of subgraphs $\langle C_\mu, C_\nu \rangle$, and $\langle C_\alpha, C_\beta \rangle$ fulfils the commutativity conditions of the Lemma 5.1.*
3. *Any pair of subgraphs $\langle C_\mu \rangle$, and $\langle C_\alpha, C_\beta \rangle$ fulfils the commutativity conditions of the corollary 5.1.*
4. *Any pair of subgraphs $\langle C_\mu \rangle$, and $\langle C_\nu \rangle$ fulfills the commutativity conditions of the corollary 5.2.*
5. *Any subgraph $\langle C_\mu, C_\nu \rangle$ satisfies the normality condition of Lemma 5.2.*

Then, the quantum state $\rho(G)$ has zero geometric quantum discord.

Proof. The proof follows from the above discussion. □

Before proceeding further, we recall a number of classes of graphs. Every vertex of a regular graph has equal degree. A complete graph has all possible edges. A bipartite graph G has two clusters C_1 and C_2 in the vertex set such that $E(G) = \{(u, v) : u \in C_1, v \in C_2\}$. That is, all the edges of a bipartite graph lies between these two clusters. A complete bipartite graph contains all such possible edges. An example of a complete bipartite graph is drawn in figure 5.2a.

Theorem 5.2. *Let G be a complete graph of order N, such that, $\rho(G) \in \mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$. Then $\rho(G)$ has no quantum discord.*

Proof. As G is a complete graph, degree of every vertex is equal $= (n - 1)$. Degree of G is $d = N(N - 1)$. Consider blocks of $\rho(G)$,

$$B_{\mu\nu} = \begin{cases} \frac{\pm 1}{d} A_{\mu\mu} = \frac{1}{d}[(N-1)I_n + J_n - I_n] = \frac{1}{d}[(N-2)I_n + J_n] & \text{for } \mu = \nu \\ \frac{\pm 1}{d} A_{\mu\nu} = \frac{\pm 1}{d} J_n & \text{for } \mu \neq \nu \end{cases}. \tag{5.57}$$

All the blocks $B_{\mu\nu}$ are normal and commute with each other. Thus, every complete graph corresponds to a zero discord quantum state. □

This theorem provides a constructive method to generate a zero discord quantum state in any given bipartite quantum system $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$. The next theorem provides an alternative to $\mathcal{H}^{(2)} \times \mathcal{H}^{(n)}$.

Theorem 5.3. *There is a quantum state $\rho(G) \in \mathcal{H}^{(2)} \times \mathcal{H}^{(n)}$ with zero discord corresponding to any complete bipartite graph $K_{n,n}$.*

Proof. Let $C_1 = \{v_{1,1}, v_{1,2}, \dots v_{1,n}\}$, $C_2 = \{v_{2,1}, v_{2,2}, \dots v_{2,n}\}$ be bipartition of $K_{n,n}$. Now,

$$\rho(K_{n,n}) = \frac{1}{2n^2} \begin{bmatrix} nI_n & \pm J_n \\ \pm J_n & nI_n \end{bmatrix}. \tag{5.58}$$

Here, all the block matrices commute with each other and they are normal matrices. Hence, $\rho(K_{n,n})$ is a quantum state with zero discord. □

(a) Graph with zero discord

(b) Graph with non-zero discord

Figure 5.2 : Two isomorphic copies of $K_{3,3}$ with zero and non-zero discord

Note that, quantum state with zero discord depends on vertex labelling. Consider isomorphic copies of $K_{3,3}$ depicted in figure 5.2. The graph in 5.2a has zero discord but, the graph in 5.2b has non-zero discord.

Consider a binary matrix $A = (a_{ij})_{n\times n}$, such that, $\sum_i a_{ij} = \sum_j a_{ij} = r$ for all i, and j. Hence, for all i and j we have $\sum a_{i*} = \sum a_{*j}$. Using the graph theoretic conversion, in the graph $\mathcal{A} = \langle C_\mu, C_\nu \rangle$, we have $\text{nbd}(v_{\mu i}) = \text{nbd}(v_{\nu j})$ for any two i and j. It indicates that $\mathcal{A}$ is a regular graph. In mathematical terminology, $\frac{1}{r}A$ is a doubly stochastic matrix .

There are 2^{n^2} binary matrices of order n. Among them, $2^{\frac{n(n+1)}{2}}$ matrices are symmetric. Excluding zero matrix from them, there are $2^{\frac{n(n+1)}{2}} - 1$ quantum states with zero discord in $\mathcal{H}^{(2)} \otimes \mathcal{H}^{(n)}$ represented by $\rho(G)$ where G is a bipartite partially symmetric graph as stated in the above theorem.

Theorem 5.4. *Let $\mathcal{A} = \langle C_\mu, C_\nu \rangle$ be a regular graph satisfying the condition of Lemma 5.2. Then $\rho(\mathcal{A})$ is a quantum state with zero discord.*

Proof. Graphs satisfying the above theorem will generate the quantum state,

$$\rho(G) = \frac{1}{2nr}\begin{bmatrix} rI_n & \pm A_n \\ \pm A_n^\dagger & rI_n \end{bmatrix} = \frac{1}{2n}\begin{bmatrix} I_n & \pm\frac{1}{r}A_n \\ \pm\frac{1}{r}A_n^\dagger & I_n \end{bmatrix}. \tag{5.59}$$

Here, A_n is a normal matrix with equal row and column sum r, which commutes with all other blocks. Therefore, $\rho(\mathcal{A})$ is a quantum state with zero discord. □

We end up this section with an example of a separable graph Laplacian quantum state having non-zero quantum discord. Recall the definition 4.4 of partially symmetric graphs. For a partially symmetric graph every block $A_{\mu\nu}$ of its adjacency matrix is symmetric. In the Chapter 3, we have discussed that under some conditions partial symmetric graphs are separable states. Now we like to state:

Example 5.3. *Consider the partially symmetric graph depicted in the figure 5.3. Clearly, it represents a separable two-qubit mixed state. Its density matrix is given by,*

$$\rho(G) = \frac{1}{6}\begin{bmatrix} 2 & 0 & -1 & -1 \\ 0 & 1 & -1 & 0 \\ -1 & -1 & 2 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}. \tag{5.60}$$

Note that, $\begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}$ *and* $\begin{bmatrix} -1 & -1 \\ -1 & 0 \end{bmatrix}$ *do not commute. Therefore, $\rho(G)$ has non-zero discord. It is easy to find a number of other such examples.*

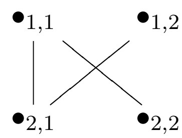


Figure 5.3 : A graph representing a separable state with non-zero discord

5.3.2 Quantum discord in graph Laplacian quantum states related to simple graphs

In the last section, we have justified that zero quantum discord is a property of combinatorial graphs. Hence, it can be measured with a number of structural constrains of graphs. We have shown if a graph G corresponds to quantum states with zero discord, then its subgraphs $\langle C_\mu \rangle$ and $\langle C_\mu, C_\nu \rangle$ fulfil five properties for all μ, ν with $1 \leq \mu, \nu \leq m$. When a graph fails to satisfy those properties, we have measured its dispersion with the quantities 'P' (5.44), 'Q' (5.45), 'R' (5.50), and 'S' (5.56).

Note that, P, Q, R and S are non-negative integers. If the graph corresponds to a classical quantum state, that is, a quantum state with zero discord, then all these quantities become zero. A function $\mathcal{M}(x, y, z, w) : \mathbb{R}^4 \to \mathbb{R}^+ \cup \{0\}$, such that, $\mathcal{M}(0, 0, 0, 0) = 0$ is called a non-negative function. Here, $\mathbb{R}^+ \cup \{0\}$ is the set of non-negative real numbers. Any suitably chosen positive function of P, Q, R and S will generate a measure of quantum correlation.

A general measure, $\mathcal{M}$, of quantum correlation is expected to possess the following properties [Streltsov, 2014, Section 4.2.2].

1. $\mathcal{M}$ is non-negative.

2. $\mathcal{M}$ is zero for classically correlated states.

3. $\mathcal{M}$ is invariant under local unitary transformation.

As an example we may consider, $\mathcal{M}(\rho) = P + Q + R + S$, as a measure of quantum discord. According to our construction, the first two properties of $\mathcal{M}$ is satisfied. The properties of local unitary operation is not modelled for quantum states corresponding to a combinatorial graph. Hence, whether $\mathcal{M}$ will satisfy the property 3 is not transparent. But it holds for a special case of local unitary operations, discussed below.

Permutation matrices are unitary matrices. Consider any two permutation matrices P_1 and P_2 acting on the Hilbert spaces $\mathcal{H}_A$, and $\mathcal{H}_B$. Thus, $P_1 \otimes P_2$ is a local unitary operator acting on $\mathcal{H}_A \otimes \mathcal{H}_B$. Before proceeding to the next theorem recall that, $P_1 \otimes P_2 = (P_1 \otimes I)(I \otimes P_2)$.

Theorem 5.5. *Let P_2 be a permutation matrix acting on the Hilbert space $\mathcal{H}_B$ and $\rho(G)$ be a quantum state with zero discord in the bipartite system $\mathcal{H}_A \otimes \mathcal{H}_B$. Consider a graph H, such that, $A(H) = (I \otimes P_2)A(G)(I \otimes P_2)^\dagger$. Then, $\rho(H)$ also represents a zero discord quantum state.*

Proof.

$$(I \otimes P_2)\rho(G)(I \otimes P_2)^\dagger = (I \otimes P_2)\frac{1}{d}\begin{bmatrix} D_1 \pm A_{11} & \pm A_{12} & \dots & \pm A_{1m} \\ \pm A_{21} & D_2 \pm A_{22} & \dots & \pm A_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \pm A_{m1} & \pm A_{m2} & \dots & D_m \pm A_{mm} \end{bmatrix} (I \otimes P_2)^\dagger$$

$$\text{or } (I \otimes P_2)\rho(G)(I \otimes P_2)^\dagger = \frac{1}{d}\begin{bmatrix} P_2(D_1 \pm A_{11})P_2^\dagger & \pm P_2 A_{12} P_2^\dagger & \dots & \pm P_2 A_{1m} P_2^\dagger \\ \pm P_2 A_{21} P_2^\dagger & P_2(D_2 \pm A_{22})P_2^\dagger & \dots & \pm P_2 A_{2m} P_2^\dagger \\ \vdots & \vdots & \ddots & \vdots \\ \pm P_2 A_{m1} P_2^\dagger & \pm P_2 A_{m2} P_2^\dagger & \dots & P_2(D_m \pm A_{mm})P_2^\dagger \end{bmatrix}.$$

Now recall the subgraphs $\langle C_\mu \rangle$ and $\langle C_\mu, C_\nu \rangle$ constructed after clustering on vertex set in equation (2.14). Graph isomorphism is represented by permutation matrices. Hence, the above equation can be interpreted as a graph isomorphism operation. The adjacency matrix of the new subgraph corresponding to $\langle C_\mu \rangle$, and $\langle C_\mu, C_\nu \rangle$ is given by $P_2 A_{\mu\mu} P_2^\dagger$, and $\begin{bmatrix} 0 & P_2 A_{\mu\nu} P_2^\dagger \\ P_2 A_{\mu\nu}^\dagger P_2^\dagger & 0 \end{bmatrix}$, respectively. Note that, the permutation matrix P_2 does not switch one vertex of C_μ to another vertex of C_ν. It only changes the indexes of vertices of $C\mu$ and C_ν in a similar fashion. Thus, the normality and commutativity conditions holds as earlier in the new graph. Hence, if $\rho(G)$ represents a zero quantum discord state, then $(I \otimes P_2)\rho(G)(I \otimes P_2)^\dagger$ also represents a zero quantum discord state. □

The above theorem indicates that $(I \otimes P_2)$ keeps the conditions for zero discord unaltered. Thus, there is no change in discord measure $\mathcal{M}$. To realize the action of $P_1 \otimes I$ on G we need a suitable reordering on the vertex set. In a similar fashion, we may prove $P_1 \otimes I$ keeps the discord measure unaltered. Combining them we get the discord measure $\mathcal{M}$ is unaltered by $P_1 \otimes P_2$.

5.3.3 Zero discord graph Laplacian states related to weighted digraphs

Now we generalize the results of the last sections to weighted digraphs. We shall derive conditions on the subgraphs $\langle C_\mu, C_\nu \rangle$ and $\langle C_\mu \rangle$ such that the blocks of $\rho(G)$ construct a family for commuting normal matrices. 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 5.3, and its corollaries 5.3 and 5.4. That the matrix A is normal has been discussed in the lemma 5.4. 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 5.6. *Blocks of a density matrix ρ 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 $1 \leq i, j \leq n$,*
$$\sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\beta j})} w(v_{\mu i}, v_{\nu k}) w(v_{\alpha k}, v_{\beta j}) = \sum_{k \in \text{nbd}(v_{\alpha i}) \cap \text{nbd}(v_{\nu j})} w(v_{\alpha i}, v_{\beta k}) w(v_{\mu k}, v_{\nu j}).$$

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

3. ***Degree condition*** *The graph satisfies the following two degree criterion,*

   a)
$$\begin{aligned} &\pm\big[w(v_{\nu i}, v_{\nu j})(d_{\mu i} - d_{\mu j}) + w(v_{\mu i}, v_{\mu j})(d_{\nu j} - d_{\nu i})\big] \\ &+ \sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\mu k}) w(v_{\nu k}, v_{\nu j}) \\ &- \sum_{k \in \text{nbd}(v_{\nu i}) \cap \text{nbd}(v_{\mu j})} w(v_{\nu i}, v_{\nu k}) w(v_{\mu k}, v_{\mu j}) = 0, \end{aligned} \tag{5.61}$$

b)

$$w(v_{\alpha i}, v_{\beta j})(d_{\mu i} - d_{\mu j}) \pm \Big[\sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\beta j})} w(v_{\mu i}, v_{\mu k}) w(v_{\alpha k}, v_{\beta j}) - \sum_{k \in \text{nbd}(v_{\alpha i}) \cap \text{nbd}(v_{\mu j})} w(v_{\alpha i}, v_{\beta k}) w(v_{\mu k}, v_{\mu j}) \Big] = 0. \tag{5.62}$$

Proof. The commutativity and normality conditions follow from the lemma 5.3 and 5.4 for all non-diagonal blocks. Note that, diagonal blocks are adjacency matrices of $\langle C_\mu \rangle$ which are Hermitian, hence normal. The degree condition includes all diagonal blocks in this family.

First we consider commutativity of two diagonal blocks,

$$\begin{aligned} &\frac{1}{d}(D_\mu \pm A_{\mu\mu})\frac{1}{d}(D_\nu \pm A_{\nu\nu}) = \frac{1}{d}(D_\nu \pm A_{\nu\nu})\frac{1}{d}(D_\mu \pm A_{\mu\mu}) \\ \Rightarrow &D_\mu D_\nu \pm D_\mu A_{\nu\nu} \pm A_{\mu\mu} D_\nu + A_{\mu\mu} A_{\nu\nu} = D_\nu D_\mu \pm D_\nu A_{\mu\mu} \pm A_{\nu\nu} D_\mu + A_{\nu\nu} A_{\mu\mu} \\ \Rightarrow &(A_{\mu\mu} A_{\nu\nu} - A_{\nu\nu} A_{\mu\mu}) \pm (D_\mu A_{\nu\nu} - A_{\nu\nu} D_\mu) \pm (A_{\mu\mu} D_\nu - D_\nu A_{\mu\mu}) = 0 \\ \Rightarrow &(A_{\mu\mu} A_{\nu\nu} - A_{\nu\nu} A_{\mu\mu})_{ij} \pm (D_\mu A_{\nu\nu} - A_{\nu\nu} D_\mu)_{ij} \pm (A_{\mu\mu} D_\nu - D_\nu A_{\mu\mu})_{ij} = 0. \end{aligned} \tag{5.63}$$

In terms of graphical parameters we may write,

$$(D_\mu A_{\nu\nu} - A_{\nu\nu} D_\mu)_{ij} = d_{\mu i}(A_{\nu\nu})_{ij} - (A_{\nu\nu})_{ij} d_{\mu j} = w(v_{\nu i}, v_{\nu j})(d_{\mu i} - d_{\mu j}), \tag{5.64}$$

$$(A_{\mu\mu} D_\nu - D_\nu A_{\mu\mu})_{ij} = (A_{\mu\mu})_{ij} d_{\nu j} - d_{\nu i}(A_{\nu\nu})_{ij} = w(v_{\mu i}, v_{\mu j})(d_{\nu j} - d_{\nu i}). \tag{5.65}$$

Also from the corollary 5.4,

$$(A_{\mu\mu} A_{\nu\nu} - A_{\nu\nu} A_{\mu\mu})_{ij} = \sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\mu k}) w(v_{\nu k}, v_{\nu j}) - \sum_{k \in \text{nbd}(v_{\nu i}) \cap \text{nbd}(v_{\mu j})} w(v_{\nu i}, v_{\nu k}) w(v_{\mu k}, v_{\mu j}). \tag{5.66}$$

Thus for commutativity of diagonal blocks the following degree condition need to be satisfied,

$$\sum_{k \in \text{nbd}(v_{\mu i}) \cap \text{nbd}(v_{\nu j})} w(v_{\mu i}, v_{\mu k}) w(v_{\nu k}, v_{\nu j}) - \sum_{k \in \text{nbd}(v_{\nu i}) \cap \text{nbd}(v_{\mu j})} w(v_{\nu i}, v_{\nu k}) w(v_{\mu k}, v_{\mu j}) \pm \big[w(v_{\nu i}, v_{\nu j})(d_{\mu i} - d_{\mu j}) + w(v_{\mu i}, v_{\mu j})(d_{\nu j} - d_{\nu i}) \big] = 0. \tag{5.67}$$

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.

$$\begin{aligned} &\frac{1}{d}(D_\mu \pm A_{\mu\mu})\frac{\pm 1}{d} A_{\alpha\beta} = \frac{\pm 1}{d} A_{\alpha\beta} \frac{1}{d}(D_\mu \pm A_{\mu\mu}) \\ \Rightarrow &D_\mu A_{\alpha\beta} \pm A_{\mu\mu} A_{\alpha\beta} = A_{\alpha\beta} D_\mu \pm A_{\alpha\beta} A_{\mu\mu}. \end{aligned} \tag{5.68}$$

Rearranging the terms we get the equation,

$$(D_\mu A_{\alpha\beta} - A_{\alpha\beta} D_\mu) \pm (A_{\mu\mu} A_{\alpha\beta} - A_{\alpha\beta} A_{\mu\mu}) = 0. \tag{5.69}$$

The above equation holds if for all i, j with $1 \leq i, j \leq n$,

$$\begin{aligned} &(D_\mu A_{\alpha\beta})_{ij} - (A_{\alpha\beta} D_\mu)_{ij} \pm \{(A_{\mu\mu} A_{\alpha\beta})_{ij} - (A_{\alpha\beta} A_{\mu\mu})_{ij}\} = 0 \\ \Rightarrow &d_{\mu i}(A_{\alpha\beta})_{ij} - (A_{\alpha\beta})_{ij} d_{\mu j} \pm \{(A_{\mu\mu} A_{\alpha\beta})_{ij} - (A_{\alpha\beta} A_{\mu\mu})_{ij}\} = 0. \end{aligned} \tag{5.70}$$

Graph theoretic counterpart of $(A_{\mu\mu}A_{\alpha\beta} - A_{\alpha\beta}A_{\mu\mu})$ follows from the corollary 5.3. Thus,

$$\begin{aligned}&(A_{\mu\mu}A_{\alpha\beta})_{ij} - (A_{\alpha\beta}A_{\mu\mu})_{ij} = \\ &\sum_{k\in \text{nbd}(v_{\mu i})\cap \text{nbd}(v_{\beta j})} w(v_{\mu i}, v_{\mu k})w(v_{\alpha k}, v_{\beta j}) - \sum_{k\in \text{nbd}(v_{\alpha i})\cap \text{nbd}(v_{\mu j})} w(v_{\alpha i}, v_{\beta k})w(v_{\mu k}, v_{\mu j}).\end{aligned} \tag{5.71}$$

Also,

$$d_{\mu i}(A_{\alpha\beta})_{ij} - (A_{\alpha\beta})_{ij}d_{\mu j} = w(v_{\alpha i}, v_{\beta j})(d_{\mu i} - d_{\mu j}). \tag{5.72}$$

Combining the above two equations we get,

$$\begin{aligned}w(v_{\alpha i}, v_{\beta j})(d_{\mu i} - d_{\mu j}) \pm \Big[&\sum_{k\in \text{nbd}(v_{\mu i})\cap \text{nbd}(v_{\beta j})} w(v_{\mu i}, v_{\mu k})w(v_{\alpha k}, v_{\beta j}) \\ &- \sum_{k\in \text{nbd}(v_{\alpha i})\cap \text{nbd}(v_{\mu j})} w(v_{\alpha i}, v_{\beta k})w(v_{\mu k}, v_{\mu j})\Big] = 0.\end{aligned} \tag{5.73}$$

□

We now make a number of observations. If vertices of $C_\mu, \mu = 1, 2, \dots m$ 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 5.3.

Also if the subgraphs $\langle C_\mu \rangle$ and $\langle C_\nu \rangle$ fulfil the commutativity condition described in the corollary 5.4 then the first degree condition takes the following simpler form:

$$w(v_{\nu i}, v_{\nu j})(d_{\mu i} - d_{\mu j}) + w(v_{\mu i}, v_{\mu j})(d_{\nu j} - d_{\nu i}) = 0 \text{ for all } i, j. \tag{5.74}$$

Further, if the subgraphs $\langle C_\alpha, C_\beta \rangle$ and $\langle C_\mu \rangle$ satisfy the commutativity condition described in the corollary 5.3, the equation is simplified to

$$w(v_{\alpha i}, v_{\beta j})(d_{\mu i} - d_{\mu j}) = 0 \text{ for all } i, j. \tag{5.75}$$

5.4 DISCORD OF SOME SPECIFIC GRAPH LAPLACIAN QUANTUM STATES

We find out conditions on graphs such that the corresponding quantum states have non-zero discord. These conditions shed light into the nature of discord in a number of important quantum states, and will be discussed in this section. Hence just by observing the structural properties of the graph, the zero or non zero discord quantum states can be determined. These properties include existence or non-existence of some particular edges, and degree of vertices. Therefore, this work develops a new method of approaching the problem of discord by exploiting the connection between graph theory and quantum mechanics. We apply these results on some important pure two qubit states, as well as a number of mixed quantum states, such as the Werner, Isotropic, and X-states.

5.4.1 Two qubit pure states

Two qubit quantum states are the simplest bipartite quantum states. Here, we consider two examples of 2-qubit pure states: $|\psi_1\rangle = a|00\rangle + b|11\rangle$, and $|\psi_2\rangle = a|00\rangle + b|01\rangle$, where $|a|^2 + |b|^2 = 1$. Restricting a and b in $|\psi_1\rangle$ to $\frac{1}{\sqrt{2}}$ leads to the well known Bell state. The density matrices corresponding to these quantum states are

$$\sigma_1 = |\psi_1\rangle\langle\psi_1| = \begin{bmatrix} a^2 & 0 & 0 & ab \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ ab & 0 & 0 & b^2 \end{bmatrix}, \text{ and } \sigma_2 = |\psi_2\rangle\langle\psi_2| = \begin{bmatrix} a^2 & ab & 0 & 0 \\ ab & b^2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{5.76}$$

(a) Graph G_1 **(b)** Graph G_2

Figure 5.4 : Graphs representing two qubit quantum states. $\rho(G_1)$ has non-zero discord but $\rho(G_2)$ has zero discord.

From basis assumptions 2.1, we can see that these density matrices represent graph Laplacian quantum states if $a^2 \geq ab$ and $b^2 \geq ab$. If $a \neq 0$ and $b \neq 0$ then these two inequalities together imply $a = b$. A density matrix of order 4 corresponds to a graph with four vertices. Also, the graphs representing 2-qubit bipartite states must have two clusters.

Example 5.4. *Consider the graphs in the figure 5.4. Their density matrices $\rho_q(G_1)$, and $\rho_q(G_2)$ are of the form σ_1, and σ_2, respectively. From the conditions in Theorem 5.6, we conclude that the graph G_1 violates the normality condition. But, the graph G_2 satisfies all of them. Hence, the state σ_2 has zero discord, but σ_1 has non-zero discord. This example clearly indicates that quantum discord of states depend on the distribution of edges in the graph.*

5.4.2 Werner state

We have considered Werner states [Werner, 1989] as Graph Laplacian quantum states in subsection 2.3.4. A Werner state is represented by (recall equation (2.26)),

$$\rho_{x,d} = \frac{d-x}{d^3-d} I + \frac{xd-1}{d^3-d} F, \tag{5.77}$$

where $F = \sum_{i,j}^{d} |i\rangle\langle j| \otimes |j\rangle\langle i|$, $x \in [0,1]$ and d is the dimention of the individual subsystems. Note that, $\rho_{x,d}$ is a real symmetric matrix of order d^2. Writing the Werner state in the equation (2.26) as a matrix we conclude that, it can be represented by a graph having a number of specific combinatorial structures. We have depicted graphs representing Werner states $\rho_{x,3}$ and $\rho_{x,4}$ in the figure 2.11. There are separable Werner states with non-zero quantum discord [Luo, 2008].

Theorem 5.7. *Every Werner state represented by a simple graph has non-zero discord.*

Proof. Note that, for all x there is only one edge in the subgraph $\langle C_\mu, C_\nu \rangle$. Its position does not vary with x. Thus forgetting the edge weight we may consider $\langle C_\mu, C_\nu \rangle$ as a simple graph. From the structure of $\langle C_\mu, C_\nu \rangle$ using the lemma 5.2, we may conclude that $A_{\mu,\nu}$ is not a normal matrix. Thus every Werner state has a non-zero discord. □

Theorem 5.8. *Graph Laplacian Werner states represented by weighted graphs have non-zero quantum discord except for a finite set of values of x.*

Proof. Note that, for all x there is only an edge $(v_{\mu,i}, v_{i,\mu})$ in the subgraph $\langle C_\mu, C_i \rangle$ where $\mu \neq i$. After the lemma 5.4 we have shown such type of graphs cannot fulfil normality condition. As an example, consider the sub-digraph $\langle C_1, C_2 \rangle$ of $\rho_{x,3}$ depicted in figure 5.5. 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, $w(v_{12}, v_{21}) w(v_{2,1} v_{1,2}) = (3x-1)^2$ but $w(v_{22}, v_{12}) w(v_{12}, v_{12}) = 0$ as v_{22} is an isolated

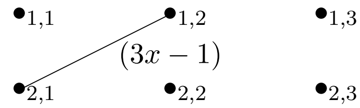


Figure 5.5 : Subgraph $\langle C_1, C_2\rangle$ of the graph representing a Werner state $\rho_{x,3}$ drawn in figure 2.11

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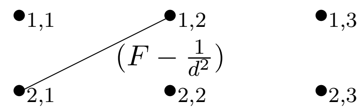


Figure 5.6 : Subgraph $\langle C_1, C_2\rangle$ of the graph representing an isotropic state $\rho_{3,x}$ drawn in the figure 2.12

vertex. In this case, the graph $\langle C_1, C_2\rangle$ fulfils the normality condition if and only if $x = \frac{1}{3}$. Thus, the normality condition of the theorem 5.6 is violated except some parameter values. Hence, graph Laplacian Werner states have non-zero quantum discord except for some values of x. □

5.4.3 Isotropic state

We have discussed about the Isotropic states in the subsection 2.3.5. Recall that, an isotropic state $\rho_{d,x}$ acting on $\mathcal{H}^{(d)} \otimes \mathcal{H}^{(d)}$ is defined by,

$$\rho_{d,x} = \frac{d^2}{d^2-1}\left[\frac{(1-F)}{d^2} I + \left(F - \frac{1}{d^2}\right) P\right], \tag{5.78}$$

where $F \in [0, 1]$ is the fidelity of the quantum state and $P = |\psi\rangle\langle\psi|$ where $|\psi\rangle = \frac{1}{\sqrt{d}}\sum_i |i_a\rangle |i_b\rangle$, the maximally entangled state in dimension d. There are graphs with a particular combinatorial structure that represent isotropic states. We have depicted graphs in the figure 2.12 representing isotropic states $\rho_{d,x}$ for $d = 2, 3, 4$. Discord of isotropic state is studied in [Luo and Fu, 2010; Guo, 2016]. Considering diagonal and off-diagonal terms we may conclude that an isotropic quantum state is graphical provided

$$(d-1)\left|F - \frac{1}{d^2}\right| \leq \frac{d^2-1}{d^2} F. \tag{5.79}$$

Putting $d = 2, 3, 4$ in the above equation we get, $\frac{1}{7} \leq F \leq 1$, $\frac{1}{13} \leq F \leq \frac{1}{5}$, $\frac{1}{11} \leq F \leq \frac{1}{21}$, respectively.

Theorem 5.9. *Graph Laplacian isotropic states have non-zero quantum discord except for some specific values of F.*

Proof. From the graph structure of the state ρ, Eq. (2.27), 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. For example consider the subgraph $\langle C_1, C_2\rangle$ of the graph $\rho_{3,x}$ depicted in the figure 5.6. 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 theorem 5.8. Thus, we may conclude that graph Laplacian isotropic states have non-zero quantum discord except for some specific values of F. □

5.4.4 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 [Ali et al., 2010; Sabapathy and Simon, 2013]. We have considered graph Laplacian X-states acting on $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$ in the subsection 2.3.6, and depicted some of the graphs representing them.

Theorem 5.10. *A graph Laplacian X state acting on $\mathcal{H}^{(m)} \otimes \mathcal{H}^{(n)}$ represented by a simple graph has zero quantum discord if and only if the following conditions are satisfied:*

1. *Any two non-empty sub-digraphs of the form $\langle C_\mu, C_\nu \rangle$ are equal.*
2. *Degree of the vertices of C_μ will fulfil $d_{\mu i} = d_{\mu(n-i)}$ for $i = 1, 2, \dots n$.*

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 5.3 we may verify that the non-empty graphs $\langle C_\mu, C_\nu \rangle$ and $\langle C_\alpha \rangle$ are commutative. Also using lemma 5.4 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,

$$w(v_{\mu i}, v_{\nu j})(d_{\alpha i} - d_{\alpha j}) = 0. \tag{5.80}$$

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

$$w(v_{\mu i}, v_{\nu(n-i)})(d_{\alpha i} - d_{\alpha(n-i)}) = 0. \tag{5.81}$$

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

Example 5.5. *Consider the graph in the figure 5.7. Let edge weight $w(v_{11}, v_{13}) = 2$ and for the other two edges, weight is 1. Here number of clusters $m = 2$ and number of vertices in each cluster $n = 3$. The corresponding quantum state is given by the density matrix,*

$$\rho(G) = \frac{1}{8}\begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 2 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 2 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}, \tag{5.82}$$

which lies in $\mathcal{H}^{(2)} \otimes \mathcal{H}^{(3)}$. Degree of the vertices are: $d(v_{11}) = 2, d(v_{12}) = 1, d(v_{13}) = 1, d(v_{11}) = 1, d(v_{22}) = 1, d(v_{23}) = 2$. According to the second condition of the above theorem, for zero discord $d(v_{11}) = d(v_{13})$ which is not fulfilled in this case. Hence, the corresponding quantum state has non-zero discord.

In general the density matrix of a two-qubit X state is given by,

$$\rho = \begin{bmatrix} \rho_{11} & 0 & 0 & \rho_{14} \\ 0 & \rho_{22} & \rho_{23} & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} \end{bmatrix}. \tag{5.83}$$

It must be a Hermitian, positive semidefinite, trace one matrix. To satisfy Hermiticity, $\rho_{41} = \overline{\rho_{14}}, \rho_{32} = \overline{\rho_{23}}$ and ρ_{ii} are real for all i. The positivity condition requires that $\rho_{22}\rho_{33} \geq |\rho_{23}|^2$ and

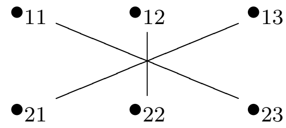


Figure 5.7 : Graph representing an X station in $\mathcal{H}^{(3)} \otimes \mathcal{H}^{(2)}$.

$\rho_{11}\rho_{44} \geq |\rho_{14}|^2$. Also, for unit trace $\sum_{i=1}^{4} \rho_{ii} = 1$. Lemma 2.1 implies that ρ represents a graph Laplacian state if and only if

$$\rho_{11} \geq |\rho_{14}|, \rho_{22} \geq |\rho_{23}|, \rho_{33} \geq |\rho_{32}| \text{ and } \rho_{44} \geq |\rho_{41}|. \tag{5.84}$$

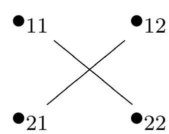
A graph with four vertices distributed into two clusters, each containing two vertices represent ρ as a graph Laplacian state. Discord of the state depends on the edge distribution in the graph. For simplicity, let the graph have no loops. Then the equation (5.84) simplifies to

$$\rho_{11} = |\rho_{14}|, \rho_{22} = |\rho_{23}|, \rho_{33} = |\rho_{32}| \text{ and } \rho_{44} = |\rho_{41}|. \tag{5.85}$$

Combining this with the positivity conditions we get,

$$\begin{aligned} \rho_{11} = |\rho_{14}| = |\rho_{41}| = \rho_{44} = a \\ \rho_{22} = |\rho_{23}| = |\rho_{32}| = \rho_{33} = b \end{aligned} \tag{5.86}$$

for some real numbers a and b. A graph satisfying the above condition is



Here, weights of (v_{11}, v_{22}) and (v_{12}, v_{21}) are a and b, respectively. Degree of the vertices are given by $d(v_{11}) = a, d(v_{12}) = b, d(v_{21}) = b$ and $d(v_{22}) = a$. Now by theorem 5.10, the corresponding quantum state has zero discord if and only if $a = b$. In all other cases ρ has non-zero discord. Further, we know that a two qubit X-state is entangled if and only if either $\rho_{22}\rho_{33} < |\rho_{14}|^2$ or $\rho_{11}\rho_{44} < |\rho_{23}|^2$. From this we can conclude that if $a = b$ then entanglement is also zero. This coincides with the results in [Ali et al., 2010].

As an important example of the above considered general two qubit X state, we take up the two qubit Werner state, given by

$$\rho = a\,|\psi^-\rangle\langle\psi^-| + \frac{1-a}{4}I, \tag{5.87}$$

where $|\psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ and $0 \leq a \leq 1$. The density matrix in expanded from is,

$$\rho = \begin{bmatrix} \frac{1-a}{4} & 0 & 0 & 0 \\ 0 & \frac{1+a}{4} & \frac{-a}{2} & 0 \\ 0 & \frac{-a}{2} & \frac{1+a}{4} & 0 \\ 0 & 0 & 0 & \frac{1-a}{4} \end{bmatrix}. \tag{5.88}$$

As $a \leq 1$, clearly $\frac{1-a}{4} \geq 0$ and $\frac{1+a}{4} \geq \frac{a}{2}$. Therefore, ρ represents a graph Laplacian quantum state for all values of a. Consider the graph shown in the figure 5.8. It represents a two qubit Werner state if loop weights are $\frac{1-a}{8}$, and edge weights are $\frac{a}{2}$. Therefore, degree of the vertices are $d(v_{11}) = \frac{1-a}{8}, d(v_{12}) = \frac{1-3a}{8}, d(v_{21}) = \frac{1-3a}{8}$ and $d(v_{22}) = \frac{1-a}{8}$. For zero discord, we need $\frac{1-a}{8} = \frac{1-3a}{8}$, which implies that $a = 0$. This is consistent with the results in [Ali et al., 2010].

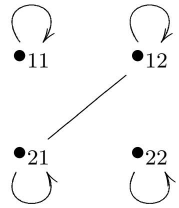


Figure 5.8 : Graph representing a two qubit Werner state

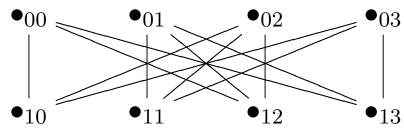


Figure 5.9 : A simple graph representing a zero discord state in $\mathcal{H}^2 \otimes \mathcal{H}^{(3)}$.

5.4.5 Graph Laplacian quantum states corresponding to simple graphs

A simple graph G satisfies the basis assumptions stated in section 2. Given any edge (i,j) of a simple graph, the edge weight $w(i,j) = w(j,i) = 1$. Also, a simple graph has no loop, that is, $(i,i) \notin E(G)$ for all vertices i. A detailed description on quantum discord of graph Laplacian quantum states arising from simple graphs is available in [Dutta et al., 2017a].

Example 5.6. *Consider the graph in figure 5.9. It has two clusters C_0 and C_1, each containing 4 vertices. Note that, there is only one bipartite subgraph $\langle C_0, C_1 \rangle$ in the above graph. Also, degree of every vertex is three. The density matrices corresponding to this graph are:*

$$\rho_l(G) = \frac{1}{24}\begin{bmatrix} 3 & 0 & 0 & 0 & -1 & 0 & -1 & -1 \\ 0 & 3 & 0 & 0 & 0 & -1 & -1 & -1 \\ 0 & 0 & 3 & 0 & -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 3 & -1 & -1 & 0 & -1 \\ -1 & 0 & -1 & -1 & 3 & 0 & 0 & 0 \\ 0 & -1 & -1 & -1 & 0 & 3 & 0 & 0 \\ -1 & -1 & -1 & 0 & 0 & 0 & 3 & 0 \\ -1 & -1 & 0 & -1 & 0 & 0 & 0 & 3 \end{bmatrix}, \text{ and } \rho_q(G) = \frac{1}{24}\begin{bmatrix} 3 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 3 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 3 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 3 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 3 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 3 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 3 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 3 \end{bmatrix}. \tag{5.89}$$

This graph satisfies all the conditions of theorem 5.1. Therefore, the mixed quantum states corresponding to this graph have zero discord.

5.5 WHAT NEXT?

In this chapter, we have studied graph theoretic criterion for graph Laplacian quantum states having zero and no-zero quantum discord. Pointer states or classical quantum states has zero quantum discord. Blocks of a density matrix of a pointer state form a family of normal commuting matrices. In this work, we exploit this condition to determine the structural properties of a graph for which this condition is met. This leads to a number of meaningful observations. We find out conditions on graphs such that the corresponding quantum states have zero discord. These conditions shed light into the nature of discord in a number of important quantum states. Hence just by observing the structural properties of the graph, the zero or non zero discord quantum states can be determined. These properties include existence or non-existence of some particular edges, and degree of vertices. Therefore, this work develops a new method of approaching the problem of discord by exploiting the connection between graph theory and quantum mechanics. We have also produced a graph theoretic measure of quantum discord for graph Laplacian quantum states related to simple graphs. There are a number of problems that can be attempted in future. Some of them are listed below:

1. Given a binary (0, 1) matrix A of order n there is a graph $\mathcal{A}$ of order $2n$ whose adjacency matrix is given by,

$$A(\mathcal{A}) = \begin{bmatrix} 0 & A \\ A^{\dagger} & 0 \end{bmatrix}. \tag{5.90}$$

   We have to find conditions on $\mathcal{A}$ such that the matrix A is a binary normal matrix. Similarly, we may construct graphs for binary normal matrices whose elements are $(1, -1)$ or $(1, 0, -1)$. Given a natural number n let number of normal binary $(0, 1), (1, -1), (1, 0, -1)$ matrix are a_n, b_n, and c_n, respectively. The sequence $\{a_{n\geq 2}\} = \{2, 8, 68, 1124, 36112, 2263268, 281249824, \dots\}$, $\{b_{n\geq 2}\} = \{2, 12, 80, 2096, 49792, 3449088, 357236224, \dots\}$ and $\{c_{n\geq 2}\} = \{3, 33, 939, 75041, 15901363, \dots\}$. Detailed description of a_n, b_n, and c_n is available in `http://oeis.org/A055547`, `http://oeis.org/A055548`, and `http://oeis.org/A055549`, respectively. But, there is no general form of these sequences. One may attempt to construct a general formula with our graph theoretic criterion for binary normal matrix.

2. We have proposed a graph theoretic measure of discord applicable for graph Laplacian quantum states related to simple graphs. In theorem 5.5, we have shown that measure is invariant under the operation $P_1 \otimes P_2$, where P_1 and P_2 are permutation matrices, which are special cases of unitary matrices. We need to prove it for arbitrary unitary matrices U_1 and U_2. But a graph theoretic description of a general local unitary operator on graphs is not known as yet. Further work is required for getting a clearer picture.