

A Graph-Theoretical Framework to Analyse Zero Discord Quantum States

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Abstract

This article comprehensively explores matrices and their prerequisites for achieving positive semi-definiteness. The study delves into a series of theorems concerning pure quantum states in the context of weighted graphs. The main objective of this study is to establish a graph-theoretic framework for the study of quantum discord and to identify the necessary and sufficient conditions for zero quantum discord states using unitary operators. This research aims to advance the understanding of quantum discord and its implications for quantum information theory with a graph-theoretic framework.

Key words: Graph Laplacian, Density operator, Quantum gates, Quantum discord

1 Introduction

In the bipartite and multipartite quantum systems, the phenomenon of entanglement exhibits that a local measurement on one subsystem will have a profound impact on the other subsystem due to the existence of nonlocal correlation [24, 10, 15, 1, 2, 33, 34]. However, it is worth noting that entanglement is not always a prerequisite for demonstrating nonlocal characteristics in quantum systems [3, 4]. For example, a quantum computing framework- deterministic quantum computation using single qubit- utilizing highly mixed states was proposed in 1998 [20, 7]. Notably, this model was successfully implemented experimentally in 2008 [21], and serves as an excellent illustration that certain highly mixed states, even when separable, exhibit intrinsic non-classical correlations which hold promising potential for applications in quantum computing. Moreover, investigations have revealed that quantum correlation exhibits greater resilience than entanglement in the presence of noise, rendering quantum algorithms relying solely on nonlocal correlations more robust compared to those relying on entanglement [32, 31, 30, 11].

Quantum discord is a measure of non-classical quantum correlation, and it has been extensively studied for achieving efficient, secure, and optimal quantum communication beyond the scope of entanglement. Quantifying quantum correlation in a bipartite state is achieved by measuring quantum discord, initially introduced by Ollivier and Zurek [26]. Obtaining an analytical expression of quantum discord for arbitrary two-qubit states is challenging due to the complex optimization over local measurements. Hence, determining whether a quantum state has zero quantum discord is crucial in distinguishing its quantum characteristics. For instance, it has been established that a vanishing quantum discord between the principal system and its surroundings is necessary and sufficient for characterizing the system's dynamics through a completely positive map [29, 22, 6, 23, 28]. Recently, researchers proposed a necessary and sufficient condition for nonzero quantum discord using singular value decomposition of a correlation matrix [6, 8, 27].

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This study presents a simplified method for assessing zero quantum discord, which involves partitioning the density matrix into block matrices and evaluating the specific properties of these blocks. Mathematically, the density operator ρ_G is defined as [13, 5, 19, 17]:

$$\rho_G = \frac{1}{\text{Tr}(L(G))} [L(G)]$$

where $L(G)$ represents the Laplacian matrix of the weighted graph G .

Since the density operator ρ_G serves as an alternate representation of the state of a quantum system, it is pivotal in understanding the evolution of quantum systems, which are inherently unitary operations. Consequently, unitary operators, often called quantum gates, play a fundamental role in quantum physics. These gates, including single-qubit gates like the Pauli operators ($\sigma_x, \sigma_y, \sigma_z$), as well as multi-qubit gates, are crucial for manipulating and transforming quantum states [25]. Notably, unitary operators enable the exploration of both separability and quantum discord, which are measures of the correlation between two subsystems of a quantum system. Ensuring the validity and reliability of quantum computations requires necessary conditions for a positive semi-definite matrix. These conditions encompass various mathematical criteria that must be satisfied by the matrix elements [14].

Condition for positive semi-definite matrix: Let $A = [a_{pq}]_{n \times n}$ be a positive semi-definite matrix then

1. $|a_{ii}| \geq \sum_{i \neq j} |a_{ij}|$ [17].
2. $\det \begin{pmatrix} a_{pp} & a_{pq} \\ a_{qp} & a_{qq} \end{pmatrix} \geq 0$ for $q > p$ [17].

Converse is true if $\begin{bmatrix} \bar{x}_p & \bar{x}_q \end{bmatrix} \begin{bmatrix} a_{pp} & a_{pq} \\ a_{qp} & a_{qq} \end{bmatrix} \begin{bmatrix} x_p \\ x_q \end{bmatrix} = |b_{pq}| |x_p + (-1)^{m_{pq}} x_q|^2 + |c_{pq}| |x_p + (-1)^{n_{pq}} i x_q|^2 + [a_{pp} - |b_{pq}| - |c_{pq}|] |x_p|^2 + [a_{qq} - |b_{pq}| - |c_{pq}|] |x_q|^2 \geq 0$ for $q > p$, here m_{pq} and n_{pq} are either odd or even and $|b_{pq}|$ and $|c_{pq}|$ are positive,

and $\begin{bmatrix} \bar{x}_p & \bar{x}_r \end{bmatrix} \begin{bmatrix} a_{pp} & a_{pr} \\ a_{rp} & a_{rr} \end{bmatrix} \begin{bmatrix} x_p \\ x_r \end{bmatrix} = |b_{pr}| |x_p + (-1)^{m_{pr}} x_r|^2 + |c_{pr}| |x_p + (-1)^{n_{pr}} i x_r|^2 + [a_{pp} - |b_{pr}| - |c_{pr}|] |x_p|^2 + [a_{rr} - |b_{pr}| - |c_{pr}|] |x_r|^2 \geq 0$ for $r > p$, here m_{pr} and n_{pr} are either odd or even and $|b_{pr}|$ and $|c_{pr}|$ are positive.

Then there exists $\begin{bmatrix} \bar{x}_q & \bar{x}_r \end{bmatrix} \begin{bmatrix} a_{qq} & a_{qr} \\ a_{rq} & a_{rr} \end{bmatrix} \begin{bmatrix} x_q \\ x_r \end{bmatrix} = b_1 |x_q + (-1)^{m_{qr}} x_r|^2 + b_2 |x_q + (-1)^{m_{pq} + n_{pr}} i x_r|^2 + b_3 |x_q + (-1)^{n_{pq} + m_{pr}} i x_r|^2 + b_4 |x_q + (-1)^{n_{pq} + n_{pr}} i i x_r|^2 + (+ve)$, where $b_1, b_2, b_3,$ and $b_4 \geq 0$ and m_{qr} is either odd or even and $m_{qr} = m_{pq} + m_{pr}$, such that $\sum \begin{bmatrix} \bar{x}_p & \bar{x}_q \end{bmatrix} \begin{bmatrix} a_{pp} & a_{pq} \\ a_{qp} & a_{qq} \end{bmatrix} \begin{bmatrix} x_p \\ x_q \end{bmatrix} = a_1 |x_1 \pm x_2 \pm \dots \pm x_n|^2 + a_2 |x_1 \pm i x_2 \pm \dots \pm i x_n|^2 + (+ve)$ which clearly shows that the matrix A is a positive semi definite matrix.

Quantum Gates: Quantum gates display reversibility, ensuring that each input has a unique corresponding output within the reversible circuit. In the realm of quantum computing, a variety of gates exists, including single-qubit gates (SQG) such as $I_2, \sigma_x, \sigma_y, \sigma_z$, and $H = \frac{1}{\sqrt{2}}[\sigma_x + \sigma_z]$, as well as multiqubit gates (MQG) such as Controlled-NOT (CX= $\begin{bmatrix} I_2 & 0 & 0 & \sigma_x \end{bmatrix}$), Controlled-Z (CZ= $\begin{bmatrix} I_2 & 0 & 0 & \sigma_z \end{bmatrix}$), and Swap gates. Combining these single and multiqubit gates effectively enables global quantum computation [9, 12]. The impact of their operations on qubits are briefly described below:

1. **Performing quantum gates on the graph:** Consider a graph G with vertices $V(G) = \{v_1, v_2, \dots, v_n\}$ and edges $E(G) = \{e_{11}, e_{12}, \dots, e_{nn}\}$. The vertices can be represented as column vectors (b_i). Applying a quantum gate to a graph G signifies the action of applying the quantum gate to individual vertices or edges.
2. **Performing quantum gate operations on a density operator:** The expression $\rho_G = \frac{1}{\text{Tr}(L)} [l_{ij} b_i \otimes b_j^T]_{2^n \times 2^n}$ represents the density operator, where $\text{Tr}(L)$ is the trace of matrix L , l_{ij} is an element of matrix L , and b_i and b_j are basis vectors, then $\rho_G \xrightarrow{\text{QG}} \rho' = \frac{1}{\text{Tr}(L)} [l_{ij} (\text{QG} \times b_i \otimes (\text{QG} \times b_j)^T)]_{2^n \times 2^n}$

3. **Partial quantum gate on a graph G [18]:** Consider a graph G with 2^n vertices. Let V be the collection of vertices, defined as $V = \{b_i = c_1^i \otimes c_2^i \otimes \cdots \otimes c_n^i \text{ for all } i = 1, 2, \dots, 2^n\}$, where c_i 's are column vectors in \mathbb{C}^2 . Let us consider a unitary operator $U = I_2 \otimes U_2 \otimes \cdots \otimes U_n$, where U_2, \dots, U_n can be either I_2 or σ_x . In this case, a partial quantum gate on the graph can be defined as $(\text{Partial}U)G = (Ub_i, Ub_j) \in E(G_1)$ for all $(b_i, b_j) \in E(G)$, where, U_k is determined by the following conditions,

- (a) $U_k = I_2$ if $c_k^i = c_k^j$.
- (b) $U_k = \sigma_x$ if $c_k^i \neq c_k^j$.

4. **Partial quantum gate on a density operator [18]:** Let $\rho_G = \frac{1}{\text{Tr}(L(G))} [l_{ij} b_i \otimes b_j^T]_{2^n \times 2^n}$ represent the density operator of the graph G with $2^{n=p+q}$ vertices. The vertex set V is defined as $V = \{b_i = c_1^i \otimes c_2^i \otimes \cdots \otimes c_n^i \text{ for all } i = 1, 2, \dots, 2^n\}$, where c_i 's are column vectors in \mathbb{C}^2 . Let us consider a unitary operator $U = \underbrace{I_2 \otimes \cdots \otimes I_2}_q \otimes U_{q+1} \otimes \cdots \otimes U_{q+p}$ such that U_{q+1}, \dots, U_{q+p} are either I_2 or σ_x and ρ_G represents as a block matrix of dimensions $2^q \times 2^q$. In this case, a partial quantum gate on the density operator can be expressed as $(\text{Partial}U)\rho_G = \frac{1}{\text{Tr}(L(G))} [l_{ij} U b_i \otimes (U b_j)^T]_{2^n \times 2^n}$, where, U_k is determined by the following conditions,

- (a) $U_k = I_2$ if $c_k^i = c_k^j$.
- (b) $U_k = \sigma_x$ if $c_k^i \neq c_k^j$.

In this article, we will adhere to the established definitions as:

1. Consider (G, a) as a graph linked to the n -qubit quantum state, consisting of 2^n ($n = p + q$) vertices labeled as (ij) , where i varies from 1 to 2^p , and j varies from 1 to 2^q .
2. The expression $|x|$ represents the absolute value of x .
3. For a matrix A , \bar{A} represents as a conjugate of A .

The article is structured as follows: Section 2 introduces a series of theorems about pure quantum states linked to weighted graphs. Section 3 delves into the concept of discord and its intricate definition within the quantum realm. It further analyzes quantum discord, unraveling its underlying characteristics and implications from a graph-theoretic perspective. In Section 4, we present a conclusive summary, highlighting the significance of our research and its potential contributions to the evolving landscape of quantum information science.

2 Conditions for a positive semi-definite matrix and the pure state associated with a weighted graph

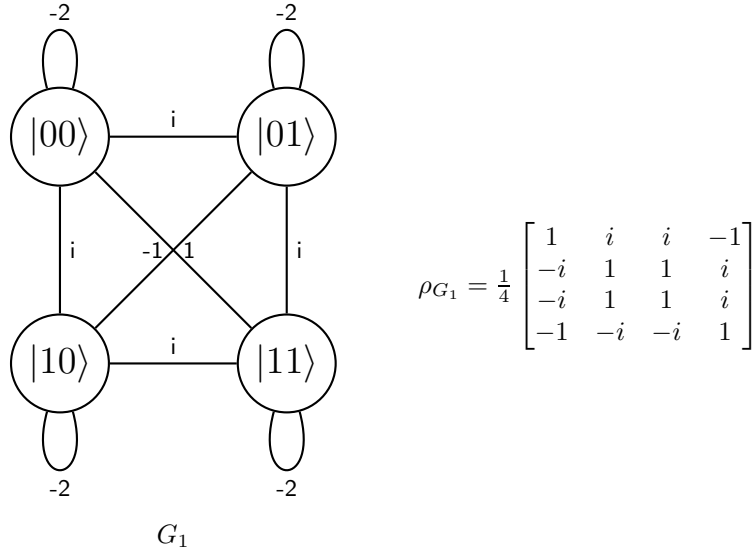
In this section, we establish a set of theorems that are presented for pure states associated with weighted graphs.

Theorem 2.1. *Let (G, a) be a connected weighted graph, which represents an m -qubit state. A state (G, a) is considered to be a pure state if the absolute value of l_{ij} is equal to d_{ii} for all values of i and j .*

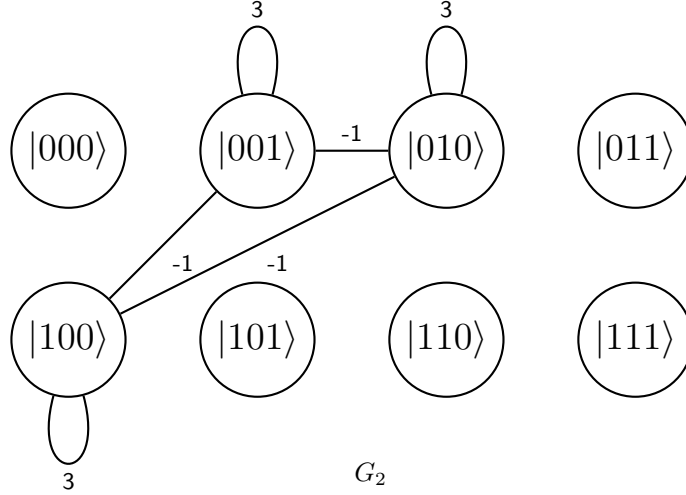
Proof: Consider (G, a) as a connected weighted graph, which represents an m -qubit state and $\rho_G = \frac{1}{\text{Tr}(L(G))} L(G) = \frac{1}{\text{Tr}(L(G))} \begin{bmatrix} d_{11} & l_{12} & \cdot & \cdot & \cdot & l_{12^m} \\ l_{21} & d_{22} & \cdot & \cdot & \cdot & l_{22^m} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ l_{2^m 1} & l_{2^m 2} & \cdot & \cdot & \cdot & d_{2^m 2^m} \end{bmatrix}$ be the density operator. If $|l_{ij}| = d_{ii} \forall i, j$, then we

clearly have $\text{Tr}(\rho_G^2) = 1$. Hence proved.

Example: The graphs G_1 and G_2 shown below also exemplify the theorem mentioned earlier.



Here $d_{11} = d_{22} = d_{33} = d_{44} = 1$, $l_{12} = l_{13} = l_{24} = l_{34} = i$, $l_{14} = l_{41} = -1$, $l_{21} = l_{31} = l_{42} = l_{43} = -i$ and $l_{23} = l_{32} = 1$. Clearly, we have $d_{ii} = |l_{ij}|$.



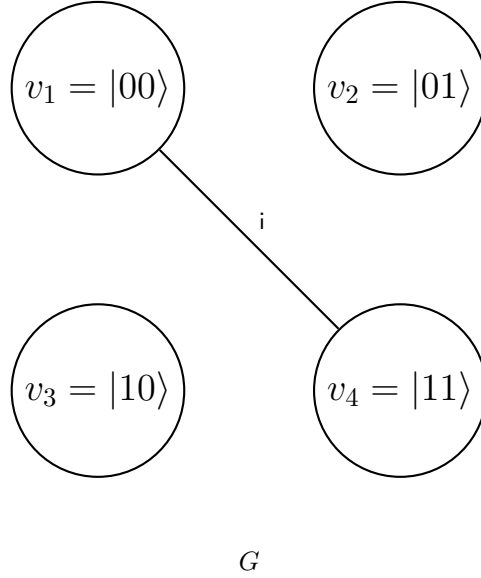
which further supports the above theorem.

Theorem 2.2. Consider a weighted graph (G, a) with 2^m vertices, where $a \in \mathbb{C}$. This graph is associated with an m -qubit state that has more than two components. If the graph consists of only one connected component,

labeled as G_1 , and each vertex in G_1 is linked to every other vertex via unique edges, satisfying the condition $|a(v_i, v_j)| = a(v_i, v_i) + \sum_{v_i \neq v_j} |a(v_i, v_j)|$ for all $v_i, v_j \in G_1$, then, the weighted graph (G, a) corresponds to a pure quantum state.

Proof: Let (G, a) ($a \in \mathbb{C}$) be a weighted graph with 2^m vertices, which represents an m -qubit quantum state. Let G_1 be the connected component of G that consists of k vertices and absolute value of edge weight $(a(v_i, v_j), \text{ for } v_i \neq v_j)$ is c . Suppose $|a(v_i, v_j)| = a(v_i, v_i) + \sum_{v_i \neq v_j} |a(v_i, v_j)|$ for all $v_i, v_j \in G_1$ which implies that diagonal sum of density operator is kc , and the diagonal entries of ρ_G^2 is kc^2 . Therefore $Tr(\rho_G^2) = 1$. Therefore, it has been demonstrated.

Example: The graph G depicted below serves as an illustration of theorem 2.2.



$$\rho_G = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -i & 0 & 0 & 1 \end{bmatrix}$$

Here connected component say G_1 is with vertex set $V = \{v_1, v_4\}$ and $a(v_1, v_1) = a(v_4, v_4) = 0$, $a(v_1, v_4) = i$.

We can see that $|a(v_1, v_4)| = a(v_1, v_1) + \sum_{v_i \neq v_j} |a(v_i, v_j)|$

Corollary 2.2.1. Consider a connected weighted graph (G, a) with 2^m vertices, associated with an m -qubit state. The weight of each edge is represented by a real number a . If the absolute of the weight of an edge from vertex v_i to v_j (where $v_i \neq v_j$) is equal to the total of the weights of all edges connected to vertex v_i , for all pairs of vertices v_i and v_j , then the weighted graph (G, a) represents the pure state.

3 Quantum Discord of weighted Graphs

In this section, we discuss various conditions for zero or nonzero quantum discord in the associated weighted graphs using block density operators.

Theorem 3.1. Consider the density operator $\rho_G = [\rho_{ij}]_{4 \times 4}$, which represents a weighted graph (G, a) on $\mathbb{C}^2 \otimes \mathbb{C}^2$. Given that U is a unitary operator expressed as $U = I_2 \otimes U_2$. If $(\overline{\text{Partial}U})\rho_G = \rho_G$ and $(\rho_{11} - \rho_{22})\rho_{14} = \rho_{12}(\rho_{13} - \rho_{24})$ then quantum discord of the weighted graph, $D_Q(G, a) = 0$.

Proof: Let (G, a) be a weighted graph defined on $\mathbb{C}^2 \otimes \mathbb{C}^2$ and $\rho_G = [\rho_{ij}]_{4 \times 4}$ represents the density operator. Clearly, $\overline{(\text{Partial}U)\rho_G} = \rho_G$ implies that blocks in the density operator are Hermitian matrices. Moreover, $(\rho_{11} - \rho_{22})\rho_{14} = \rho_{12}(\rho_{13} - \rho_{24})$ reveals commutativity of the blocks as expressed by $\rho_{11}\rho_{14} + \rho_{12}\rho_{24} = \rho_{12}\rho_{13} + \rho_{22}\rho_{14}$. Hence the proof [16].

Example: Let $\rho = \frac{1}{4}[I + \sum_{i=1}^3 T_{ii}\sigma_i \otimes \sigma_i]$ be a density operator. The quantum discord for the density matrix ρ is equal to zero if $T_{22} = T_{33} = 0$ [6, 35].

$$\rho = \frac{1}{4}[I + \sum_{i=1}^3 T_{ii}\sigma_i \otimes \sigma_i] = \frac{1}{4} \begin{bmatrix} 1 + T_{33} & 0 & 0 & T_{11} - T_{22} \\ 0 & 1 - T_{33} & T_{11} + T_{22} & 0 \\ 0 & T_{11} + T_{22} & 1 - T_{33} & 0 \\ T_{11} - T_{22} & 0 & 0 & 1 + T_{33} \end{bmatrix}$$

As per the Theorem 3.1 $\overline{(\text{Partial}U)\rho_G} = \rho_G$ if $T_{11} - T_{22} = T_{11} + T_{22}$ which implies $T_{22} = 0$. Also for $\rho_{11}\rho_{14} + \rho_{12}\rho_{24} = \rho_{12}\rho_{13} + \rho_{22}\rho_{14}$, one can show $(1 + T_{33})(T_{11} - T_{22}) = (1 - T_{33})(T_{11} - T_{22})$. For $T_{22} = 0$, $T_{11} + T_{33}T_{11} = T_{11} - T_{33}T_{11}$ or $2T_{33}(T_{11}) = 0$ which implies that $T_{33} = 0$.

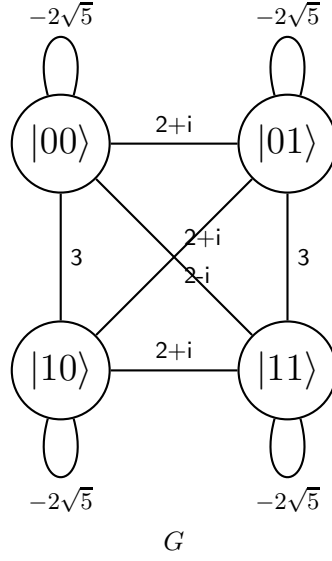
Corollary 3.1.1. Let ρ_G represent the density operator of a weighted graph (G, a) on $\mathbb{C}^2 \otimes \mathbb{C}^2$. The quantum discord $D_Q(G, a) = 0$ if $(I_2 \otimes \sigma_x)\rho_G = \rho_G$ and $(\sigma_x \otimes I_2)\rho_G = \rho_G$.

Proof: Let ρ_G represent the density operator of a weighted graph (G, a) on $\mathbb{C}^2 \otimes \mathbb{C}^2$, given by $\rho_G = \begin{bmatrix} A & B \\ B^* & C \end{bmatrix}$. The conditions $\overline{(I_2 \otimes \sigma_x)\rho_G} = \rho_G$ and $(\sigma_x \otimes I_2)\rho_G = \rho_G$ show that each block is in the form $\begin{bmatrix} a & ib \\ -ib & a \end{bmatrix}$ and $\rho_{11} - \rho_{22} = \rho_{13} - \rho_{24} = 0$. Using these results, one can easily show that blocks are commuting with each other. [16].

Theorem 3.2. Let ρ_G represent the density operator corresponding to a weighted graph (G, a) . Suppose the graph is associated with an n -qubit state ($n = p + q$) such that $\rho_G = [A^{xy}]_{2^q \times 2^q}$ ($A^{xy} = [a_{ij}^{xy}]_{2^p \times 2^p}$). The density operator ρ_G can recursively represented as the block matrices such as $A^{xy} = B^{xy} - C^{xy} + iD^{xy} - iE^{xy}$ where B^{xy}, C^{xy}, D^{xy} , and $E^{xy} \geq 0$. The quantum discord $D_Q(G, a) = 0$ if $B^{lm}, B^{rs}, C^{lm}, C^{rs}, D^{lm}, D^{rs}, E^{lm}$, and E^{rs} all commute with each other, for all lm and rs where $A^{rs} = B^{rs} - C^{rs} + iD^{rs} - iE^{rs}$ with B^{rs}, C^{rs}, D^{rs} , and $E^{rs} \geq 0$, and $A^{lm} = B^{lm} - C^{lm} + iD^{lm} - iE^{lm}$ where B^{lm}, C^{lm}, D^{lm} , and $E^{lm} \geq 0$.

Proof: Consider ρ_G as the density operator corresponding to a weighted graph (G, a) . Let us assume the graph is associated with an n -qubit state, and ρ_G can be represented as a block matrix $\rho_G = [A^{xy}]_{2^q \times 2^q}$, where $A^{xy} = [a_{ij}^{xy}]_{2^p \times 2^p}$. Assume that $A^{lm} = B^{lm} - C^{lm} + iD^{lm} - iE^{lm}$, where B^{lm}, C^{lm}, D^{lm} , and E^{lm} are positive semi-definite matrices and $A^{rs} = B^{rs} - C^{rs} + iD^{rs} - iE^{rs}$ where B^{rs}, C^{rs}, D^{rs} , and E^{rs} are positive semi-definite matrices. If $B^{lm}, B^{rs}, C^{lm}, C^{rs}, D^{lm}, D^{rs}, E^{lm}$, and E^{rs} all commute with each other, for all lm and rs , then $A^{lm}A^{rs} = (B^{lm} - C^{lm} + iD^{lm} - iE^{lm})(B^{rs} - C^{rs} + iD^{rs} - iE^{rs}) = (B^{lm} - C^{lm} + iD^{lm} - iE^{lm})(B^{rs}) - (B^{lm} - C^{lm} + iD^{lm} - iE^{lm})(C^{rs}) + i(B^{lm} - C^{lm} + iD^{lm} - iE^{lm})(D^{rs}) - i(B^{lm} - C^{lm} + iD^{lm} - iE^{lm})(E^{rs}) = (B^{rs})(B^{lm} - C^{lm} + iD^{lm} - iE^{lm}) - (C^{rs})(B^{lm} - C^{lm} + iD^{lm} - iE^{lm}) + i(D^{rs})(B^{lm} - C^{lm} + iD^{lm} - iE^{lm}) - i(E^{rs})(B^{lm} - C^{lm} + iD^{lm} - iE^{lm}) = (B^{rs} - C^{rs} + iD^{rs} - iE^{rs})(B^{lm} - C^{lm} + iD^{lm} - iE^{lm}) = A^{rs}A^{lm}$. Hence Proved [16].

Example: The graph G shown below illustrates the aforementioned theorem.



We have $\rho_G = \frac{1}{12} \begin{bmatrix} 3 & 2+i & 3 & 2+i \\ 2-i & 3 & 2-i & 3 \\ 3 & 2+i & 3 & 2+i \\ 2-i & 3 & 2-i & 3 \end{bmatrix} = \begin{bmatrix} A^{11} & A^{12} \\ A^{21} & A^{22} \end{bmatrix} = \frac{1}{3} \left\{ \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \otimes \frac{1}{2} \begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix} \right\} + \frac{2}{3} \left\{ \frac{1}{4} \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix} \otimes \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \right\}.$

Here $(\rho_{11} - \rho_{22})\rho_{14} = \rho_{12}(\rho_{13} - \rho_{24})$, $A^{11} = \frac{1}{12} \begin{bmatrix} 3 & 2+i \\ 2-i & 3 \end{bmatrix}$, $A^{12} = \frac{1}{12} \begin{bmatrix} 3 & 2+i \\ 2-i & 3 \end{bmatrix} = \frac{1}{12} \left\{ \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix} + \begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix} \right\}$,

and $A^{lm}A^{rs} = A^{rs}A^{lm}$.

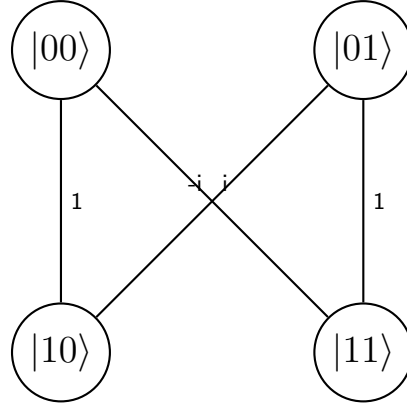
Theorem 3.3. Consider ρ_G as the density operator of a weighted graph (G, a) that is associated with an n -qubit state such that $\rho_G = [A^{xy}]_{2^q \times 2^q}$ ($A^{xy} = [a_{ij}^{xy}]_{2^p \times 2^p}$) can be represented as a block matrix. Assume $(\overline{\text{Partial}U})\rho_G = \rho_G$, where $U = \underbrace{I_2 \otimes \cdots \otimes I_2}_q \otimes \underbrace{U_{q+1} \cdots \otimes U_{q+p}}_p$, and U_i represents either I_2 or σ_x . The

quantum discord $D_Q(G, a) = 0$, if $(\overline{\text{Partial}U'})A^{rs}A^{lm} = A^{rs}A^{lm}$ for all lm and rs , where $U' = (U_1 \otimes U_2 \otimes \cdots \otimes U_p)$.

Proof: Consider ρ_G as the density operator of a weighted graph (G, a) which is associated with an n -qubit state. Assume that the density operator ρ_G can be expressed as a block matrix, denoted as $[A^{xy}]_{2^q \times 2^q}$, where each block A^{xy} is a $2^p \times 2^p$ matrix represented by $[a_{ij}^{xy}]_{2^p \times 2^p}$. Consider a unitary operator U defined as: $U = \underbrace{I_2 \otimes \cdots \otimes I_2}_q \otimes \underbrace{U_{q+1} \cdots \otimes U_{q+p}}_p$, where U_i are either I_2 or σ_x . Furthermore, if $(\overline{\text{Partial}U})\rho_G = \rho_G$, it

implies that the blocks A^{xy} being Hermitian. Now if $(\overline{\text{Partial}U'})A^{rs}A^{lm} = A^{rs}A^{lm}$ for all lm and rs , where $U' = (U_1 \otimes U_2 \otimes \cdots \otimes U_p)$ then $A^{rs}A^{lm}$ is Hermitian. Consequently, it also implies that $A^{rs}A^{lm} = A^{lm}A^{rs}$. Hence $D_Q(G, a) = 0$ [16].

Example: The graphs shown below, denoted as G_1 and G_2 , also exemplify the theorem stated above.



G_1

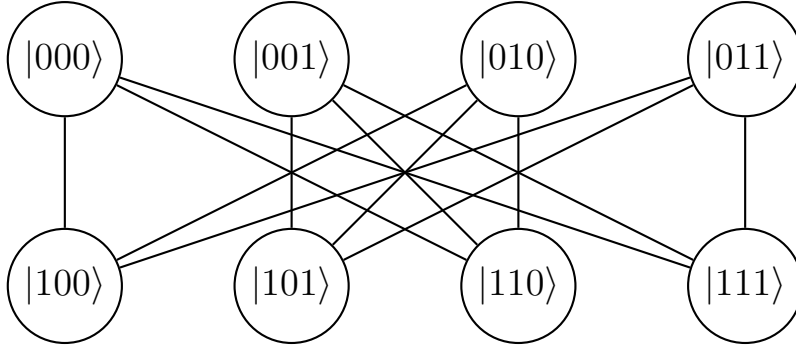
The density operator ρ_G for the graph G_1 is,

$$\rho_{G_1} = \frac{1}{8} \begin{bmatrix} 2 & 0 & 1 & -i \\ 0 & 2 & i & 1 \\ 1 & -i & 2 & 0 \\ i & 1 & 0 & 2 \end{bmatrix}$$

Here $A^{11} = \frac{1}{8} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$ and $A^{12} = \frac{1}{8} \begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix}$.

Therefore, we can show that $\overline{(PartialU')} A^{11} A^{12} = A^{11} A^{12} = \frac{1}{32} \begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix} = A^{12} A^{11}$.

Moreover, for the graph G_2



G_2

the density operator ρ_{G_2} is,

$$\rho_{G_2} = \frac{1}{24} \begin{bmatrix} 3 & 0 & 0 & 0 & -1 & 0 & -1 & -1 \\ 0 & 3 & 0 & 0 & 0 & -1 & -1 & -1 \\ 0 & 0 & 3 & 0 & -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 3 & -1 & -1 & 0 & -1 \\ -1 & 0 & -1 & -1 & 3 & 0 & 0 & 0 \\ 0 & -1 & -1 & -1 & 0 & 3 & 0 & 0 \\ -1 & -1 & -1 & 0 & 0 & 0 & 3 & 0 \\ -1 & -1 & 0 & -1 & 0 & 0 & 0 & 3 \end{bmatrix}$$

where $A^{11} = \frac{1}{24} \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix}$ and $A^{12} = \frac{1}{24} \begin{bmatrix} -1 & 0 & -1 & -1 \\ 0 & -1 & -1 & -1 \\ -1 & -1 & -1 & 0 \\ -1 & -1 & 0 & -1 \end{bmatrix}$,

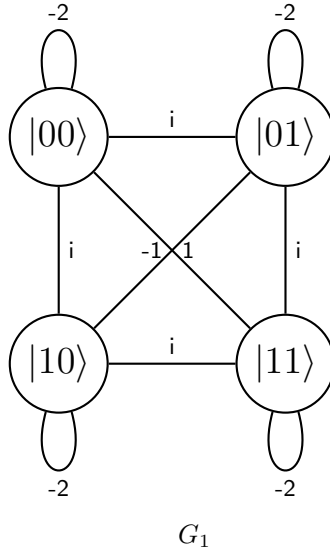
Similar to the case of G_1 , we can show that $\overline{(\text{Partial}U)}A^{11}A^{12} = A^{11}A^{12} = \frac{1}{576} \begin{bmatrix} -3 & 0 & -3 & -3 \\ 0 & -3 & -3 & -3 \\ -3 & -3 & -3 & 0 \\ -3 & -3 & 0 & -3 \end{bmatrix} =$

$A^{12}A^{11}$.

Theorem 3.4. Consider ρ_G as the density operator of a weighted graph (G, a) connected to an n -qubit state with 2^n vertices, where $\rho_G = [A^{xy}]_{2^{n-1} \times 2^{n-1}}$ ($A^{xy} = [a_{ij}^{xy}]_{2 \times 2}$). If $\rho_G = \overline{(\text{Partial}U)}\rho_G$ with $|a_{ij}^{xy}| = |a_{i_{j+1}}^{xy}|$ where $U = \underbrace{I_2 \otimes \dots \otimes I_2}_{n-1} \otimes U_n$ is a unitary operator, then the graph corresponding to the quantum state will exhibit a quantum discord value of zero.

Proof: Consider ρ_G as the density operator of a weighted graph (G, a) connected to an n -qubit state with 2^n vertices where $\rho_G = [A^{xy}]_{2^{n-1} \times 2^{n-1}}$ ($A^{xy} = [a_{ij}^{xy}]_{2 \times 2}$). Let us further introduce a unitary operators $U = \underbrace{I_2 \otimes \dots \otimes I_2}_{n-1} \otimes U_n$, where U_n is either I_2 or σ_x . For $\rho_G = \overline{(\text{Partial}U)}\rho_G$, we have all the 2-dimensional blocks A^{xy} of ρ_G as Hermitian matrices. Furthermore, if $|a_{ij}^{xy}| = |a_{i_{j+1}}^{xy}|$ then block A^{xy} either takes the form $A^{xy} = i^m \begin{bmatrix} a & ia \\ -ia & a \end{bmatrix}$ or $A^{xy} = \begin{bmatrix} a & a \\ a & a \end{bmatrix}$. Hence, the proof [16].

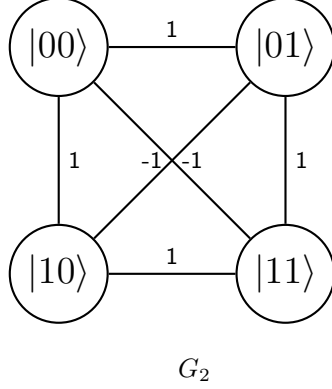
Example: The graphs illustrated below, denoted as G_1 and G_2 , also exemplify the theorem discussed above.



The density operator linked to the graph G_1 can be expressed as

$$\rho_{G_1} = \frac{1}{4} \begin{bmatrix} 1 & i & i & -1 \\ -i & 1 & 1 & i \\ -i & 1 & 1 & i \\ -1 & -i & -i & 1 \end{bmatrix}$$

Thus, $A^{11} = \frac{1}{4} \begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix}$, $A^{12} = \frac{1}{4}i \begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix}$ which shows $A^{11}A^{12} = A^{12}A^{11}$.



We can deduce the density operator associated with the graph G_2 as

$$\rho_{G_2} = \frac{1}{4} \begin{bmatrix} 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$$

Evidently, $A^{11} = \frac{1}{4} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$, $A^{12} = -\frac{1}{4} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$ indicating $A^{11}A^{12} = A^{12}A^{11}$.

Theorem 3.5. Consider (G, a) as a weighted graph with 2^n vertices, which represents an n -qubit quantum state. Let $E(G)$ be the set of edges in (G, a) , defined as

$$E(G) = \{(v_{ij}, v_{kl}); \text{ such that edge lies between } v_{ij} \text{ and } v_{kl}\}.$$

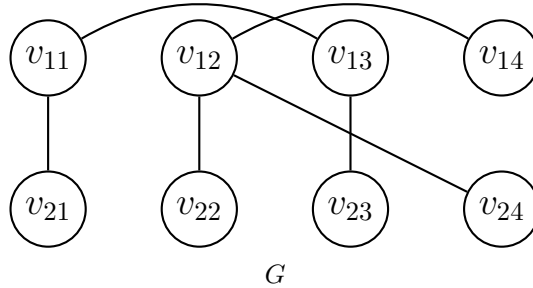
If there exists an edge (v_{ij}, v_{kl}) in graph G such that both j and l are either odd or even, then $D_Q(G, a)$, is equal to zero.

Proof: Consider (G, a) as a weighted graph with 2^n vertices, which represents an n -qubit quantum state. Let $E(G)$ be the edge set in (G, a) , defined as $E(G) = \{(v_{ij}, v_{kl}); \text{ such that edge lies between } v_{ij} \text{ and } v_{kl}\}$.

Interestingly, if (v_{ij}, v_{kl}) belongs to $E(G)$ and both j and l are either odd or even, then the density operator (ρ_G) can be expressed as a diagonal matrix in every block.

Diagonal matrices have a significant property that they commute with each other. Therefore, the blocks of the density operator (ρ_G) , being diagonal matrices, also commute. Hence, it is proved [16].

Example: The graph displayed below, represented by G , offers an illustration of the theorem mentioned earlier



The associated density operator is $\rho_G = \frac{1}{12} \begin{bmatrix} 2 & 0 & -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 3 & 0 & -1 & 0 & -1 & 0 & -1 \\ -1 & 0 & 2 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$ where each 2×2 block

are in the diagonal form.

Theorem 3.6. Consider a weighted graph (G, a) with 2^n vertices, associated with an n -qubit quantum state. Let $E(G)$ denote the set of edges in (G, a) , defined as

$$E(G) = \{(v_{ij}, v_{kl}) \text{ such that edge lies between } v_{ij} \text{ and } v_{kl}\}.$$

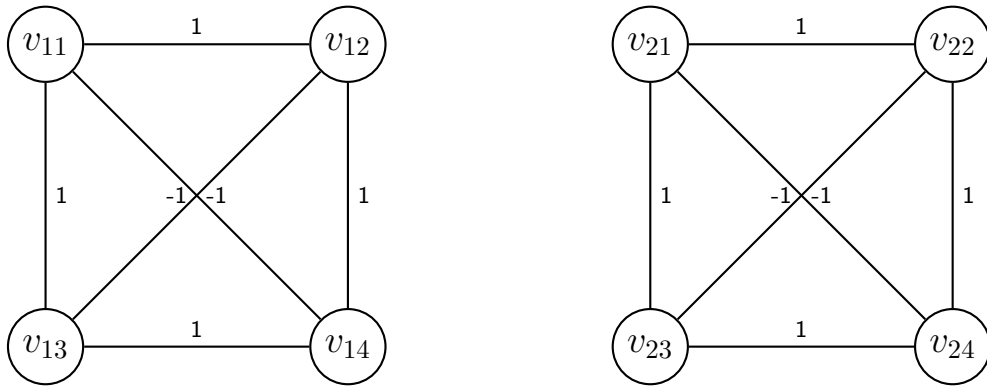
If there exists an edge (v_{ij}, v_{kl}) in the graph (G, a) for all $i = k$, then the graph (G, a) is correlated with a quantum state that has zero discord.

Proof: Consider a weighted graph (G, a) having 2^n vertices. This graph depicts a quantum state consisting of n -qubits. The set of edges of the graph (G, a) , represented as

$$E(G) = \{(v_{ij}, v_{kl}) \text{ such that edge lies between } v_{ij} \text{ and } v_{kl}\}.$$

If $i = k$, then the density operator expressed as a diagonal block matrix which linked to the graph (G, a) . Notably, these diagonal matrices in the density operator are positive semi-definite. Hence Proved. [16].

Example: Below is a graph, labeled as G , which serves as an illustrative example of the previously discussed theorem.



G

The density operator of the graph is a diagonal block matrix such that

$$\rho_G = \frac{1}{8} \begin{bmatrix} 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \end{bmatrix}$$

The proof, therefore, follows from the theorem.

Theorem 3.7. Consider $\rho_G = [A^{xy}]_{2 \times 2}$ as the density operator of a weighted graph (G, a) with 2^n vertices, related to an n -qubit quantum state. Here, A^{xy} is a block matrix defined as $A^{xy} = [A_{ij}^{xy}]_{2^{n-q-1} \times 2^{n-q-1}}$.

The quantum discord $D_Q(G, a) = 0$ if $\sum_k A_{ik}^{xy} A_{kj}^{rs} = \sum_k A_{ik}^{rs} A_{kj}^{xy}$ for all i, j and $\text{Partial}(U^i)\rho_G = \rho_G$, for $U^1 = \underbrace{I_2 \otimes \cdots \otimes I_2}_p \otimes U_{p+1} \cdots \otimes U_{p+q}$, and $U^2 = I_2 \otimes U_2 \cdots \otimes U_n$, where, U_k are either I_2 or σ_x .

Proof: Consider a weighted graph (G, a) with 2^n vertices related to an n -qubit quantum state. Let $\rho_G = [A^{xy}]_{2 \times 2}$ represent the density operator of this graph, where A^{xy} is a block matrix of size 2^{n-q-1} and A^{xy} is composed of elements denoted as A_{ij}^{xy} . If $\sum_k A_{ik}^{xy} A_{kj}^{rs} = \sum_k A_{ik}^{rs} A_{kj}^{xy}$ for all i, j and $\text{Partial}(U^i)\rho_G = \rho_G$, for $U^1 = \underbrace{I_2 \otimes \cdots \otimes I_2}_p \otimes U_{p+1} \cdots \otimes U_{p+q}$, and $U^2 = I_2 \otimes U_2 \cdots \otimes U_n$, where, U_i are either I_2 or σ_x , then A^{xy} and A^{mn} commute, and each block of A^{xy} also commutes. Hence, the discord is zero [16].

Corollary 3.7.1. Consider $\rho_G = [A^{xy}]_{4 \times 4}$ as the density operator of a weighted graph (G, a) with 2^n vertices where (G, a) represents an n -qubit quantum state, and A^{xy} be the block matrix of the density operator. The quantum discord $D_Q(G, a) = 0$ if $(A^{11} - A^{22})A^{14} = A^{12}(A^{13} - A^{24})$.

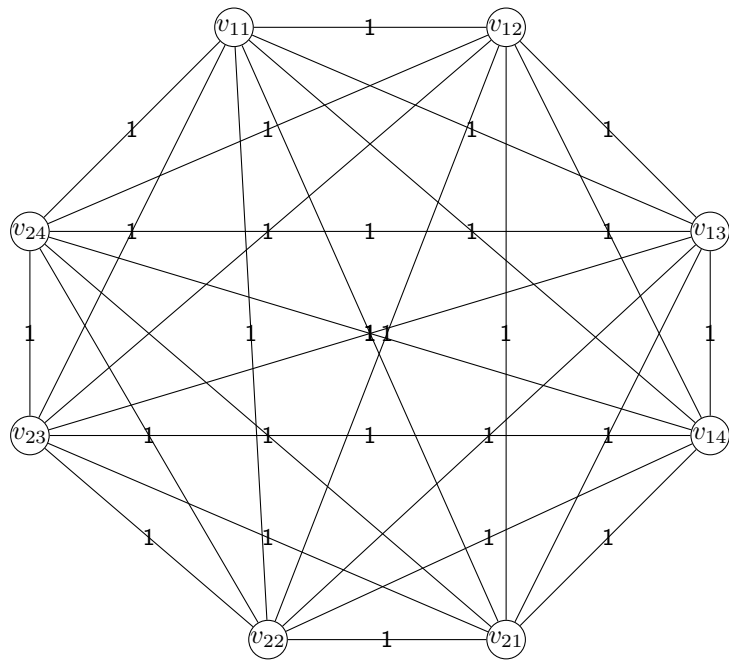
Theorem 3.8. Consider $\rho_G = [\rho_{ij}]_{2^n \times 2^n}$ as the density operator of a weighted graph (G, a) with 2^n vertices where (G, a) represents an n -qubit quantum state. The quantum discord is zero, if the density operator can be expressed as $\rho_G = \sum_i p_i \rho_i^1 \otimes \rho_i^2$, with the condition that ρ_i^1 and ρ_i^2 commute.

Proof: Consider $\rho_G = [\rho_{ij}]_{2^n \times 2^n}$ as the density operator of a weighted graph (G, a) with 2^n vertices where (G, a) represents an n -qubit quantum state. Therefore, if the density operator is written as $\rho_G = \sum_i p_i \rho_i^1 \otimes \rho_i^2$ where ρ_i^1 and ρ_i^2 commute, then the quantum discord is zero. (The normality and commutativity of blocks of the density operator imply that the quantum discord is zero [16].)

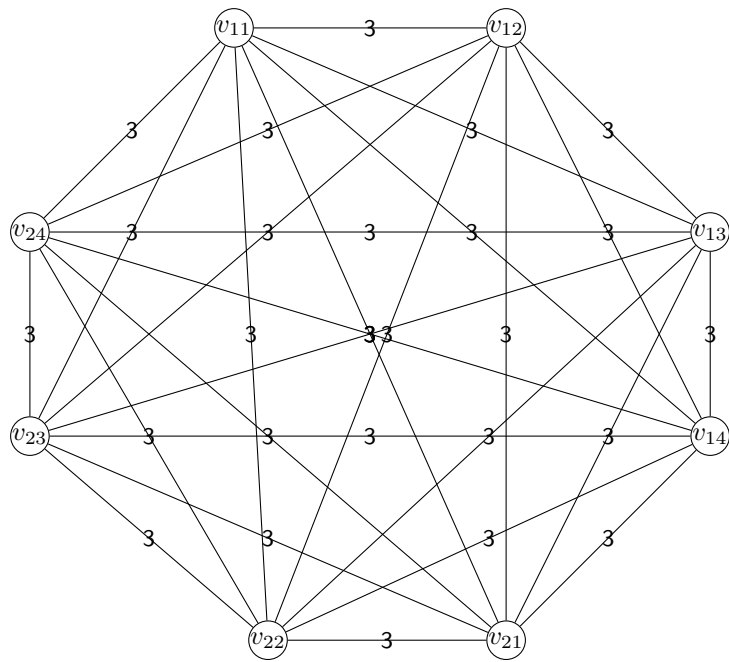
Theorem 3.9. Let (G, a) represent a weighted graph with 2^n vertices, which represents an n -qubit state. The state has zero quantum discord, if $a_{ij,kl} = b \forall (v_{ij}, v_{kl}) \in E(G)$ and $d_{ij,ij} = b(2^n - 1)$ for all v_{ij} .

Proof: Let (G, a) be a weighted graph on 2^n vertices, which represents an n -qubit state. For $a_{ij,kl} = b \forall (v_{ij}, v_{kl}) \in E(G)$ and $d_{ij,ij} = b(2^n - 1)$ for all v_{ij} , we have $a \in \mathbb{R}$ and $d_{ij,ij} = \sum a_{ij,kl}$ which illustrates that the graph (G, a) is a complete graph. Therefore, the density operator can be formulated as $\rho_G = \rho_1 \otimes \rho_2$ and all blocks commute. Thus demonstrated. [16].

Example: Here, we discuss graphs associated with a quantum state that has zero quantum discord, e.g., a complete graph, and a complete weighted graph $K(n, a)$, $a > 0$ associated with a three-qubit state.



Complete Graph (G_1)



Complete Graph with weight $a = 3$ (G_2)

Theorem 3.10. Consider ρ_G as the density operator of a weighted graph (G, a) with $n = 2^m$ vertices where (G, a) represents an n -qubit quantum state. If the reduced density operator ρ_G^A is singular, then the quantum discord of the quantum state is zero, i.e., $D_Q(G, a) = 0$.

Proof: Consider $\rho_G = [\rho_{ij}]_{2^m \times 2^m}$ as a density operator of a weighted graph (G, a) with $n = 2^m$ vertices where (G, a) represents an n -qubit quantum state.

Since $\det(\rho_G^A) = 0$, we have

$$(\rho_{11} + \dots + \rho_{\frac{n}{2}\frac{n}{2}})(\rho_{\frac{n}{2}+1\frac{n}{2}+1} + \dots + \rho_{nn}) = |(\rho_{1\frac{n}{2}+1} + \rho_{2\frac{n}{2}+2} + \dots + \rho_{\frac{n}{2}n})|^2.$$

For $\det(L^A) = 0$, it is established that the density operator can be expressed as a product state [17], where each block commutes with one another. Therefore, it has been demonstrated.

4 Conclusion

In this article, we presented a comprehensive analysis to study and characterize the properties of weighted graphs. The focus of our study revolved around the manifestation of zero discord as we presented significant findings in this area. Using a systematic approach, we divided the density matrix into distinct blocks, allowing for a thorough evaluation of zero discord across various quantum states. The outcomes of our investigation will have important implications for foundational aspects of quantum communication and computing.

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