3-regular mixed graphs with optimum Hermitian energy

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Abstract

Let $G$ be a simple undirected graph, and $G^\phi$ be a mixed graph of $G$ with the generalized orientation $\phi$ and Hermitian-adjacency matrix $H(G^\phi)$. Then $G$ is called the underlying graph of $G^\phi$. The Hermitian energy of the mixed graph $G^\phi$, denoted by $\mathcal{E}_H(G^\phi)$, is defined as the sum of all the singular values of $H(G^\phi)$. The $k$-regular mixed graph on $n$ vertices having Hermitian energy $n\sqrt{k}$ is called the $k$-regular optimum Hermitian energy mixed graph. In this paper, we first characterize all the optimum Hermitian energy mixed graphs with underlying graph hypercube. Then we focus on the problem proposed by Liu and Li [J. Liu, X. Li, Hermitian-adjacency matrices and Hermitian energies of mixed graphs, Linear Algebra Appl. 466(2015), 182–207] of determining all the 3-regular connected optimum Hermitian energy mixed graphs.

Keywords: mixed graph, Hermitian energy, Hermitian-adjacency matrix, regular graph

AMS Subject Classification Numbers: 05C20, 05C50, 05C90

1 Introduction

Let $G$ be a simple undirected graph with vertex set $V(G)$ and edge set $E(G)$. A generalized orientation $\phi$ of $G$ is to give each edge of $S$ an orientation according to $\phi$. 

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where $S \subseteq E(G)$. Then $G^\phi$ is called a mixed graph of $G$ with the generalized orientation $\phi$. If $S = E(G)$, the mixed graph $G^\phi$ is an oriented graph. If $S = \emptyset$, then $G^\phi$ is an undirected graph. Thus we find that mixed graphs incorporate both undirected graphs and oriented graphs as extreme cases. In a mixed graph $G^\phi = (V(G^\phi), E(G^\phi))$, if one element $(u, v)$ in $E(G^\phi)$ is an edge (resp. arc), we denote it by $u \leftrightarrow v$ (resp. $u \rightarrow v$). The graph $G$ is called the underlying graph of $G^\phi$. A mixed graph is called regular if its underlying graph is a regular graph. Similarly, in terms of defining order, size, degree and so on, we focus only on its underlying graph. For undefined terminology and notations, we refer the reader to [1, 3].

The Hermitian-adjacency matrix $H(G^\phi)$ of $G^\phi$ with vertex set $V(G^\phi) = \{1, 2, \ldots, n\}$ is a square matrix of order $n$, whose entry $h_{kl}$ is defined as

$$h_{kl} = \begin{cases} h_{lk} = 1, & \text{if } k \leftrightarrow l, \\ -h_{lk} = i, & \text{if } k \rightarrow l, \\ 0, & \text{otherwise,} \end{cases}$$

where $i$ is the imaginary number unit. Since $H(G^\phi)$ is a Hermitian matrix, i.e. $H(G^\phi) = [H(G^\phi)]^* := [H(G^\phi)]^T$, the eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ of $H(G^\phi)$ are all real. In [9], Liu and Li introduced the Hermitian energy of the mixed graph $G^\phi$, denoted by $\mathcal{E}_H(G^\phi)$, which is defined as the sum of the singular values of $H(G^\phi)$. Since the singular values of $H(G^\phi)$ are the absolute values of its eigenvalues, we have

$$\mathcal{E}_H(G^\phi) = \sum_{j=1}^{n} |\lambda_j|.$$

The concept of the energy of simple undirected graphs was introduced by Gutman in [5], which is related to the total $\pi$-electron energy of the molecule represented by that graph. Since then, the graph energy has been extensively studied. For more details, we refer [6, 8] to the reader.

In [9], Liu and Li gave a sharp upper bound of the Hermitian energy in terms of its order $n$ and the maximum degree $\Delta$, i.e.

$$\mathcal{E}_H(G^\phi) \leq n\sqrt{\Delta}.$$

Furthermore, they showed that the equality holds if and only if $H^2(G^\phi) = \Delta I_n$, which implies that $G^\phi$ is $\Delta$-regular. For convenience, in this paper a mixed graph on $n$ vertices with maximum degree $\Delta$ which satisfies $\mathcal{E}_H(G^\phi) = n\sqrt{\Delta}$ is called an optimum Hermitian
energy mixed graph. Let $I_n$ be the identity matrix of order $n$. For simplicity, we always write $I$ when its order is clear from the context. It is important to determine a family of $k$-regular mixed graphs with optimum Hermitian energy for any positive integer $k$. In [9], Liu and Li gave $Q_k$ a suitable generalized orientation such that it has optimum Hermitian energy. Besides, they proposed the following problem:

**Problem 1.1** Determine all the $k$-regular mixed graphs $G^\phi$ on $n$ vertices with $\mathcal{E}_H(G^\phi) = n\sqrt{k}$ for each $k$, $3 \leq k \leq n$.

Liu and Li [9] showed that a 1-regular connected mixed graph on $n$ vertices has optimum Hermitian energy if and only if it is an edge or arc. At the same time, they also proved that a 2-regular connected mixed graph on $n$ vertices has optimum Hermitian energy if and only if it is one of the three types of mixed 4-cycles. If $G^\phi_1$ and $G^\phi_2$ are two $k$-regular mixed graphs with optimum Hermitian energy, then so is their disjoint union. Thus, we only consider $k$-regular connected mixed graphs.

In this paper, we firstly show that the optimum Hermitian energy mixed graphs with underlying graph hypercube are unique (up to switching equivalence). Afterwards, we characterize all 3-regular connected optimum Hermitian energy mixed graphs, which (up to switching equivalence) in fact are only two special graphs. Thus we solve Problem 1.1 for $k = 3$.

## 2 Preliminaries

In this section, we give some notations and known results. Besides, we also introduce the definition of switching equivalence.

Let $G = G(V, E)$ be a graph with vertex set $V$ and edge set $E$. For any $v \in V$, we denote the neighborhood of $v$ by $N_G(v)$ in $G$. Let $G[S]$ denote the subgraph of $G$ induced by $S$, where $S \subseteq V$. In addition, we give $G$ a generalized orientation $\phi$. Then we get a mixed graph denoted by $G^\phi = (V(G^\phi), E(G^\phi))$ and the Hermitian-adjacency matrix $H(G^\phi)$ of $G^\phi$.

In [9], Liu and Li gave a sharp upper bound for the Hermitian energy of a mixed graph and a necessary and sufficient condition to attain the upper bound.

**Lemma 2.1** ([9, part of Theorem 3.2]). Let $G^\phi$ be a mixed graph on $n$ vertices with maximum degree $\Delta$. Then $\mathcal{E}_H(G^\phi) \leq n\sqrt{\Delta}$. 

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Lemma 2.2 (9, part of Corollary 3.3). Let $H$ be the Hermitian-adjacency matrix of a mixed graph $G^\phi$ on $n$ vertices. Then $E_H(G^\phi) = n\sqrt{\Delta}$ if and only if $H^2 = \Delta I_n$, i.e. the inner products $H(u,:) \cdot H(v,:) = 0$, $H(:,u) \cdot H(:,v) = 0$ for different vertices $u$ and $v$ of $G^\phi$, where $H(u,:)$ and $H(:,u)$ represent row vector and column vector corresponding to vertex $u$ in $H(G^\phi)$, respectively.

Moreover, Liu and Li [9] gave a characterization of the $k$-regular connected optimum Hermitian energy mixed graphs.

Lemma 2.3 (9, part of Lemma 3.5). Let $G^\phi$ be a $k$-regular connected mixed graph with order $n$ ($n \geq 3$), then $E_H(G^\phi) = n\sqrt{k}$ if and only if for any pair of vertices $u$ and $v$ with distance not more than two in $G$ such that $N(u) \cap N(v) \neq \emptyset$, there are edge-disjoint mixed 4-cycles $uxvy$ of the following three types; see Fig.2.1.

![Figure 2.1: Three types of mixed 4-cycles.](image)

By Lemma 2.2, if $G^\phi$ is a connected mixed graph on $n$ vertices with optimum Hermitian energy $n\sqrt{\Delta}$, then $G^\phi$ is $\Delta$-regular. Moreover, since any two distinct rows of $H$ are orthogonal, we can deduce the following lemma.

Lemma 2.4 Let $H$ be the Hermitian-adjacency matrix of a $k$-regular mixed graph $G^\phi$ on $n$ vertices. If $H^2 = kI_n$, then $|N(u) \cap N(v)|$ is even for pair of vertices $u$ and $v$ with distance no more than two.

Next we introduce the definition of switching equivalence. Let $G^\phi$ be a mixed graph with vertex set $V$. The switching function of $G^\phi$ is a function $\theta : V \to T$, where $T = \{1, -1, i, -i\}$. The switching matrix of $G^\phi$ is a diagonal matrix $D(\theta) := \text{diag}(\theta(v_k) : v_k \in V)$, where $\theta$ is a switching function. Let $G^{\phi_1}, G^{\phi_2}$ and $G^{\phi_3}$ be three mixed graphs with the same underlying graph $G$ and vertex set $V$. If there exists a switching matrix $D(\theta)$ such that $H(G^{\phi_2}) = D(\theta)^{-1}H(G^{\phi_1})D(\theta)$, then we say $G^{\phi_1}$ and $G^{\phi_2}$ are switching equivalent, denoted by $G^{\phi_1} \sim G^{\phi_2}$. If two mixed graphs $G^{\phi_1}$ and $G^{\phi_2}$ are switching equivalent, then $Sp_H(G^{\phi_1}) = Sp_H(G^{\phi_2})$ i.e. $E_H(G^{\phi_1}) = E_H(G^{\phi_2})$. Moreover, if $G^{\phi_1} \sim G^{\phi_2}$ and $G^{\phi_2} \sim G^{\phi_3}$, then $G^{\phi_1} \sim G^{\phi_3}$.
Note that Liu and Li [9] also introduced the definition of switching equivalence between mixed graphs. However, $T = \{1, i, -i\}$ in their definition. Besides, our definition coincides with the definition of switching equivalence between oriented graphs which is given in [2] when the mixed graphs are oriented graphs.

3 Main results

In this section, we firstly prove that all the $k$-regular connected optimum Hermitian energy mixed graphs with underlying graph hypercube are switching equivalent. That is the optimum Hermitian energy mixed graphs with underlying graph hypercube are unique (up to switching equivalence) for any positive integer $k$. And then we characterize all 3-regular connected optimum Hermitian energy mixed graphs (up to switching equivalence).

Firstly, we give the following definition about hypercube $Q_k$ which can be found in [7].

Definition 3.1 [7] A hypercube $Q_k$ of dimension $k$ is defined recursively in terms of the Cartesian product of graphs as follows

$$Q_k = \begin{cases} 
K_2, & k = 1, \\
Q_{k-1} \square Q_1, & k \geq 2. 
\end{cases}$$

Lemma 3.2 Let $Q_k^\phi$ be a mixed graph with the generalized orientation $\phi$. Then $Q_k^\phi$ has optimum Hermitian energy if and only if every mixed 4-cycle in $Q_k^\phi$ is one of the three types in Fig 2.1.

Proof. For any two distinct vertices $u$ and $v$ of $Q_k$, we know that $|N(u) \cap N(v)|$ is either zero or two, where $N(\cdot)$ stands for the neighborhood of a vertex in $Q_k$. Thus, if there is one common neighbor between the two vertices in $Q_k^\phi$, then they have exactly two common neighbors $x$ and $y$ i.e. there is exactly one mixed 4-cycle $uxvy$. By Lemma 2.3, it is easy to obtain this lemma.

Hypercube $Q_k$ is a very important family of graphs and it has many nice properties. Liu and Li [9] gave $Q_k$ a suitable generalized orientation such that it has optimum Hermitian energy. Now we give $Q_k$ a new generalized orientation $\phi_0$. For convenience, we assume that the vertex set of $Q_k$ is $\{1, 2, \ldots, 2^{k-1}, 2^{k-1} + 1, 2^{k-1} + 2, \ldots, 2^k\}$ with $G[V_1] = G[V_2] = Q_{k-1}$, where $V_1 = \{1, 2, \ldots, 2^{k-1}\}, V_2 = \{2^{k-1} + 1, 2^{k-1} + 2, \ldots, 2^k\}$. Firstly, we give the hypercube $Q_1$ a generalized orientation $Q_1^{\phi_0}$ such that $1 \rightarrow 2$. Afterwards, we suppose that $Q_{k-1}$ has been oriented into $Q_{k-1}^{\phi_0}$. By reversing every arc of $Q_{k-1}^{\phi_0}$,
we can get another new generalized orientation denoted by $-\phi_0$. For $Q_k$, we give $G[V_1]$ the generalized orientation $\phi_0$ and $G[V_2]$ the generalized orientation $-\phi_0$. Next we put an arc from each vertex in $G[V_1]$ to the corresponding vertex in $G[V_2]$ i.e. $t \to 2^{k-1} + t$ for $t = 1, 2, \ldots, 2^{k-1}$. Then we get $Q_k^{\phi_0}$.

![Figure 3.2: The first three mixed hypercubes $Q_1^{\phi_0}, Q_2^{\phi_0}, Q_3^{\phi_0}$.](image)

The lemma below shows that the Hermitian energy of $Q_k^{\phi_0}$ is optimum.

**Lemma 3.3** Let $Q_k$ be a hypercube of dimension $k$ with $n = 2^k$ vertices. Then $Q_k^{\phi_0}$ satisfies $H^2(Q_k^{\phi_0}) = kI_n$ (or $E_H(Q_k^{\phi_0}) = n\sqrt{k}$).

**Proof.** If $k = 1$, then

$$H(Q_k^{\phi_0}) = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}.$$ 

Hence it is easy to show that $H^2(Q_1^{\phi_0}) = I_2$ and we only need to consider the case $k \geq 2$.

By Lemma 3.2 if every mixed 4-cycle of $Q_k^{\phi_0}$ is the third mixed 4-cycle in Fig 2.1 then $E_H(Q_k^{\phi_0}) = n\sqrt{k}$. Therefore, we just need to show that every mixed 4-cycle of $Q_k^{\phi_0}$ is the third mixed 4-cycle in Fig 2.1 for $k \geq 2$. We shall apply induction on $k$. If $k = 2$, $Q_2^{\phi_0}$ is the third mixed 4-cycle in Fig 2.1. Suppose now that $k > 2$ and the lemma holds for fewer $k$. Then every mixed 4-cycle of $Q_k^{\phi_0}$ is the third mixed 4-cycle in Fig 2.1 and so is $Q_{k-1}^{\phi_0}$.

Moreover by the definition of $Q_k^{\phi_0}$, we have

$$H(Q_k^{\phi_0}) = \begin{bmatrix} H(Q_{k-1}^{\phi_0}) & iI \\ -iI & H(Q_{k-1}^{-\phi_0}) \end{bmatrix}.$$ 

For any mixed 4-cycle of $Q_k^{\phi_0}$, if it is contained by the induced subgraph $G[V_1]$ or $G[V_2]$, then we can get that it is the third mixed 4-cycle in Fig 2.1 by the induction hypothesis.
Thus, we just talk about the 4-cycle $C$ induced by \(\{s, t, t + 2^{k-1}, s + 2^{k-1}\}\), where $1 \leq s < t \leq 2^{k-1}$. If $s \rightarrow t$ in $Q^\phi_k$, then $s + 2^{k-1} \leftrightarrow t + 2^{k-1}$, $s \rightarrow s + 2^{k-1}$ and $t \rightarrow t + 2^{k-1}$. It is easy to see that the mixed 4-cycle $C$ is the third mixed 4-cycle in Fig. 2.1. Above all, we get that every mixed 4-cycle of $Q^\phi_k$ is the third mixed 4-cycle in Fig. 2.1 for $k \geq 2$. Thus, We complete the proof.

**Theorem 3.4** Let $Q_k^\phi$ be an optimum Hermitian energy mixed graph with underlying graph $Q_k$. Then $Q_k^\phi$ is unique (up to switching equivalence) for any positive integer $k$.

**Proof.** We shall apply induction on $k$. If $k = 1$, $Q_k^\phi$ is an edge $Q_1$ or an arc $Q_1^\phi$. Then

\[
H(Q_1) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad H(Q_1^\phi) = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}.
\]

It is easy to find the switching matrix $D(\theta) = \begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix}$ such that $H(Q_1) = D^{-1}(\theta)H(Q_1^\phi)D(\theta)$. Hence, $Q_1 \sim Q_1^\phi$. Namely $Q_k^\phi$ is unique (up to switching equivalence) for $k = 1$. Now we assume that the theorem holds for fewer $k$.

Let $Q_k^\phi$ be a mixed graph with optimum Hermitian energy. For the sake of convenience, assume that $V(Q_k^\phi) = \{1, 2, \ldots, 2^{k-1}, 2^{k-1} + 1, 2^{k-1} + 2, \ldots, 2^k\}$ such that both $G[V_1]$ and $G[V_2]$ are mixed graphs with underlying graph $Q_{k-1}$, where $V_1 = \{1, 2, \ldots, 2^{k-1}\}$, $V_2 = \{2^{k-1} + 1, 2^{k-1} + 2, \ldots, 2^k\}$. From Lemma 3.2, we know that every mixed 4-cycle in $Q_k^\phi$ is one of the three types in Fig. 2.1. Then every mixed 4-cycle in $G[V_1]$ and $G[V_2]$ is one of the three types in Fig. 2.1. By Lemma 3.2, $G[V_1]$ and $G[V_2]$ have optimum Hermitian energy. Thus, we have

\[
H(Q_k^\phi) = \begin{bmatrix} H(G[V_1]) & S \\ S^* & H(G[V_2]) \end{bmatrix},
\]

where $S$ is a diagonal matrix and its diagonal element belongs to \(\{1, i, -i\}\). By the induction, we can find a switching matrix $D_1(\theta)$ such that $H(Q_{k-1}^\phi) = D_1^{-1}(\theta)H(G[V_1])D_1(\theta)$. Assume that $Q_{k-1}$ is a bipartite graph with bipartition $X$ and $Y$. Let a diagonal matrix $D_3(\theta) = diag(\theta(v_k)|\theta(v_k) = 1$, if $v_k \in X$; $\theta(v_k) = -1$, if $v_k \in Y)$. Then $H(Q_{k-1}^\phi) = D_3^{-1}(\theta)H(Q_{k-1}^\phi)D_3(\theta)$. Hence $Q_{k-1}^\phi \sim Q_{k-1}$ i.e. $Q_{k-1}^\phi$ has optimum Hermitian energy. Similarly, we can find the switching matrix $D_2(\theta)$ such that $H(Q_{k-1}^\phi) = D_2^{-1}(\theta)H(G[V_2])D_2(\theta)$ by the induction hypothesis.

Let

\[
T_1 = \begin{bmatrix} D_1(\theta) & 0 \\ 0 & I \end{bmatrix}, \quad T_2 = \begin{bmatrix} I & 0 \\ 0 & D_2(\theta) \end{bmatrix}.
\]
Then $T_1$ and $T_2$ are switching matrices and we get that

\[
T_2^{-1}T_1^{-1}H(Q_k^\phi)T_1T_2 = \begin{bmatrix} I & 0 \\ 0 & D_2(\theta) \end{bmatrix}^{-1} \begin{bmatrix} D_1(\theta) & 0 \\ 0 & I \end{bmatrix}^{-1} \begin{bmatrix} H(G[V_1]) & S \\ S^* & H(G[V_2]) \end{bmatrix}
\]

\[
\times \begin{bmatrix} D_1(\theta) & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & D_2(\theta) \end{bmatrix}
\]

\[
= \begin{bmatrix} D_1(\theta)^{-1}H(G[V_1])D_1(\theta) & D_1(\theta)^{-1}SD_2(\theta) \\ D_2(\theta)^{-1}S^*D_1(\theta) & D_2(\theta)^{-1}H(G[V_2])D_2(\theta) \end{bmatrix}
\]

\[
= \begin{bmatrix} H(Q_{k-1}^{\phi_0}) & S_1 \\ S_1^* & H(Q_{k-1}^{-\phi_0}) \end{bmatrix},
\]

where $S_1 = D_1^{-1}(\theta)SD_2(\theta) = \begin{bmatrix} s_{11} & 0 & \cdots & 0 \\ 0 & s_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & s_{2k-1,2k-1} \end{bmatrix}$ and $s_{tt} \in \{1,-1,i,-i\}$ with $1 \leq t \leq 2^{k-1}$.

Now we divide the discussion about the value of $s_{11}$ into four cases:

**Case 1.** $s_{11} = 1$.

Let

\[
T_3 = \begin{bmatrix} I & 0 \\ 0 & iI \end{bmatrix}.
\]

Then

\[
H = T_3^{-1}T_2^{-1}T_1^{-1}H(Q_k^\phi)T_1T_2T_3 = \begin{bmatrix} H(Q_{k-1}^{\phi_0}) & S_2 \\ S_2^* & H(Q_{k-1}^{-\phi_0}) \end{bmatrix},
\]

where $S_2 = I^{-1}S_1(iI) = iS_1$.

**Case 2.** $s_{11} = -1$.

Let

\[
T_3 = \begin{bmatrix} I & 0 \\ 0 & -iI \end{bmatrix}.
\]

Then

\[
H = T_3^{-1}T_2^{-1}T_1^{-1}H(Q_k^\phi)T_1T_2T_3 = \begin{bmatrix} H(Q_{k-1}^{\phi_0}) & S_2 \\ S_2^* & H(Q_{k-1}^{-\phi_0}) \end{bmatrix},
\]

where $S_2 = I^{-1}S_1(-iI) = -iS_1$. 

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Case 3. $s_{11} = i$.

Let $T_3 = I$. Then

$$H = T_3^{-1}T_2^{-1}T_1^{-1}H(Q_k^0)T_1T_2T_3 = \begin{bmatrix} H(Q_{k-1}^0) & S_2 \\ S_2^* & H(Q_{k-1}^0) \end{bmatrix},$$

where $S_2 = I^{-1}S_1(I) = S_1$.

Case 4. $s_{11} = -i$.

Let

$$T_3 = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}.$$

Then

$$H = T_3^{-1}T_2^{-1}T_1^{-1}H(Q_k^0)T_1T_2T_3 = \begin{bmatrix} H(Q_{k-1}^0) & S_2 \\ S_2^* & H(Q_{k-1}^0) \end{bmatrix},$$

where $S_2 = I^{-1}S_1(-I) = -S_1$.

Assume that $S_2 = \begin{bmatrix} s'_{11} & 0 & \cdots & 0 \\ 0 & s'_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & s'_{2k-12k-1} \end{bmatrix}$ and $H = (h_{kk})$. Then $h_{t(2^k-1)+t} = s''_{tt}$, $1 \leq t \leq 2^k-1$ and $h_{1(2^k-1+1)} = s'_{11} = i$. Let $T = T_1T_2T_3$. Then $H = T^{-1}H(Q_k^0)T$, where $T$ is a diagonal matrix and every diagonal element belongs to $\{1, -1, i, -i\}$. Since $H^2(Q_k^0) = kI$, we get that $HH^* = H^2 = kI$. Thus, the inner product of any two rows of $H$ is zero. Suppose that vertex $j$ is a neighbor of vertex 1, where $j \in V_1$. Next we consider the inner product of the first row and the $2^k-1 + j$th row in $H$. If $1 \to j$, then $h_{1j} = i, h_{(2^k-1+1)(2^k-1+j)} = -i$ and $h_{(2^k-1+j)(2^k-1+1)} = \overline{h_{(2^k-1+1)(2^k-1+j)}} = i$. Since $H(1,:) \cdot H(2^k-1+j,:) = h_{1j}h_{2^k-1+j} + h_{(2^k-1+1)h_{2^k-1+j}}(2^k-1+1) = ih_{j(2^k-1+j)} + i(-i) = 0$, we get that $h_{j(2^k-1+j)} = i$ i.e. $j \to 2^k-1+j$; see Fig.3.3(a). If $1 \leftrightarrow j$, then $h_{1j} = -i, h_{(2^k-1+1)(2^k-1+j)} = i$ and $h_{(2^k-1+j)(2^k-1+1)} = \overline{h_{(2^k-1+1)(2^k-1+j)}} = -i$. Since $H(1,:) \cdot H(2^k-1+j,:) = h_{1j}h_{2^k-1+j} + h_{1(2^k-1+1)h_{2^k-1+j}}(2^k-1+1) = (-i)h_{j(2^k-1+j)} + ii = 0$, we get that $h_{j(2^k-1+j)} = i$ i.e. $j \to 2^k-1+j$; see Fig.3.3(b). Due to the connection of $Q_{k-1}$, we can show that $h_{2(2^k-1+2)} = h_{3(2^k-1+3)} = \cdots = h_{2k-12k} = i$. Then $S_2 = iI$ and

$$H = \begin{bmatrix} H(Q_{k-1}^0) & iI \\ -iI & H(Q_{k-1}^0) \end{bmatrix} = H(Q_k^0).$$

Thus, there exists a switching matrix $D(\theta) = T$ such that $H(Q_k^0) = D(\theta)^{-1}H(Q_k^0)D(\theta)$. That is $Q_k^\phi \sim Q_k^{\phi_0}$.

Above all, we can conclude that any optimum Hermitian energy mixed graph with underlying graph $Q_k$ is unique (up to switching equivalence) for any positive integer $k$.
Figure 3.3: Two generalized orientations of edges related to vertices $1, j, 2^{k-1}+1, 2^{k-1}+j$.

The proof is complete.

In the following, we give the characterization of all 3-regular mixed graphs with optimum Hermitian energy.

Let $G^\phi$ be a 3-regular optimum Hermitian energy mixed graph. By Lemma 2.2 and Lemma 2.4, we can see that $G^\phi$ satisfies that $|N(u) \cap N(v)|$ is even for any two distinct vertices $u$ and $v$ of $G^\phi$. Then the underlying graph of $G^\phi$ with $\mathcal{E}_H(G^\phi) = n\sqrt{3}$ is either the complete graph $K_4$ or the hypercube $Q_3$ from Theorem 3.5 in [4]. Hence, we just need to consider the 3-regular optimum Hermitian energy mixed graphs with underlying graph $K_4$ or $Q_3$. Then we get the result below.

**Theorem 3.5** Let $G^\phi$ be a 3-regular optimum Hermitian energy mixed graph. Then $G^\phi$ (up to switching equivalence) is either $G_1$ or $G_2$ drawn in Fig.3.4

![Figure 3.4](image)

(a) $G_1$ 
(b) $G_2$

Figure 3.4: All 3-regular optimum Hermitian energy mixed graphs.

**Proof.** Based on the analyse above, we know that the underlying graph of the 3-regular optimum Hermitian energy mixed graph $G^\phi$ is either the complete graph $K_4$ or the hypercube $Q_3$. From Theorem 3.3, the optimum Hermitian energy mixed graphs with underlying graph $Q_3$ are switching equivalent to $G_2$ i.e. $Q_3^\phi$ drawn in Fig.3.2. Next we just consider the case that the underlying graph is the complete graph $K_4$ and divide our discussion into four cases:
Case 1. $G^\phi$ is an oriented graph.

We can deduce that $H(G^\phi) = iS(G^\phi)$. By the definitions of Hermitian energy and skew energy, we have that the Hermitian energy of $G^\phi$ is equal to its skew energy. Hence, $G^\phi$ has the optimum Hermitian energy if and only if it has the optimum skew energy. Moreover from Theorem 3.8 in [4], we obtain that $G^\phi$ (up to switching equivalence) is $G_1$ drawn in Fig. 3.

Case 2. $G^\phi$ is not an oriented graph and no vertex has two incident edges. Then there exists a vertex, say $u_1$, which has one incident edge $u_1 \leftrightarrow u_2$.

Subcase 2.1. $u_1 \rightarrow u_3$ and $u_1 \rightarrow u_4$.

By Lemma 2.2, we have $H(u_1, :) \cdot H(u_2, :) = 0$. Then $\overline{h}_{11} h_{21} + \overline{h}_{12} h_{22} + \overline{h}_{13} h_{23} + \overline{h}_{14} h_{24} = -i h_{23} - i h_{24} = 0$. Hence $h_{23} = i$, $h_{24} = -i$ or $h_{23} = -i$, $h_{24} = i$, that is, $u_2 \rightarrow u_3$, $u_2 \leftarrow u_4$ or $u_2 \leftarrow u_3$, $u_2 \rightarrow u_4$. Without loss of generality, assume that $u_2 \rightarrow u_3$, $u_2 \leftarrow u_4$. By Lemma 2.2 it follows that $H(u_1, :) \cdot H(u_3, :) = 0$. Then $\overline{h}_{11} h_{31} + \overline{h}_{12} h_{32} + \overline{h}_{13} h_{33} + \overline{h}_{14} h_{34} = -i - i h_{34} = 0$. Hence $h_{34} = -1$, which is a contradiction.

Subcase 2.2. $u_1 \leftarrow u_3$ and $u_1 \leftarrow u_4$.

By Lemma 2.2, $H(u_1, :) \cdot H(u_2, :) = 0$. Then $\overline{h}_{11} h_{21} + \overline{h}_{12} h_{22} + \overline{h}_{13} h_{23} + \overline{h}_{14} h_{24} = i h_{23} + i h_{24} = 0$. Hence $h_{23} = i$, $h_{24} = -i$ or $h_{23} = -i$, $h_{24} = i$, that is, $u_2 \rightarrow u_3$, $u_2 \leftarrow u_4$ or $u_2 \leftarrow u_3$, $u_2 \rightarrow u_4$. Without loss of generality, assume that $u_2 \rightarrow u_3$, $u_2 \leftarrow u_4$. By Lemma 2.2 it follows that $H(u_1, :) \cdot H(u_3, :) = 0$. Then $\overline{h}_{11} h_{31} + \overline{h}_{12} h_{32} + \overline{h}_{13} h_{33} + \overline{h}_{14} h_{34} = -i + i h_{34} = 0$. Hence $h_{34} = 1$ i.e. there is an edge $u_3 \leftrightarrow u_4$ in $G^\phi$. However, $H(u_1, :) \cdot H(u_4, :) = \overline{h}_{11} h_{41} + \overline{h}_{12} h_{42} + \overline{h}_{13} h_{43} + \overline{h}_{14} h_{44} = i + i \neq 0$, which is a contradiction.

Subcase 2.3. $u_1 \rightarrow u_3$, $u_1 \leftrightarrow u_4$ or $u_1 \leftarrow u_3$, $u_1 \rightarrow u_4$.

Without loss of generality, assume that $u_1 \rightarrow u_3$ and $u_1 \leftrightarrow u_4$. By a similar way, we can prove that this subcase could not happen.

Case 3. No vertex has three incident edges, and there exists a vertex, say $u_1$, has two incident edges $u_1 \leftrightarrow u_2$ and $u_1 \leftrightarrow u_3$. Then for the vertex $u_4$, there is an arc $u_1 \rightarrow u_4$ or $u_1 \leftarrow u_4$.

Suppose that $u_1 \rightarrow u_4$. By Lemma 2.2 we have $H(u_1, :) \cdot H(u_2, :) = 0$. Then $\overline{h}_{11} h_{21} + \overline{h}_{12} h_{22} + \overline{h}_{13} h_{23} + \overline{h}_{14} h_{24} = h_{23} - i h_{24} = 0$. Hence $h_{23} = 1$, $h_{24} = -i$ or $h_{23} = i$, $h_{24} = 1$, that is, $u_2 \leftrightarrow u_3$, $u_2 \leftarrow u_4$ or $u_2 \rightarrow u_3$, $u_2 \leftrightarrow u_4$. If $u_2 \leftrightarrow u_3$, $u_2 \leftrightarrow u_4$, then $H(u_1, :) \cdot H(u_3, :) = 0$ from Lemma 2.2. It implies that $\overline{h}_{11} h_{31} + \overline{h}_{12} h_{32} + \overline{h}_{13} h_{33} + \overline{h}_{14} h_{34} = 1 - i h_{34} = 0$. Thus $h_{34} = -i$ i.e. $u_3 \leftrightarrow u_4$. However, $H(u_1, :) \cdot H(u_4, :) = \overline{h}_{11} h_{41} + \overline{h}_{12} h_{42} + \overline{h}_{13} h_{43} + \overline{h}_{14} h_{44} = i + i \neq 0$, which is a contradiction. If $u_2 \rightarrow u_3$, $u_2 \leftrightarrow u_4$, then $H(u_1, :) \cdot H(u_3, :) = 0$ from Lemma 2.2. It implies that $\overline{h}_{11} h_{31} + \overline{h}_{12} h_{32} + \overline{h}_{13} h_{33} + \overline{h}_{14} h_{34} = -i - i h_{34} = 0$. Thus
\( h_{34} = -1 \), which is a contradiction.

For \( u_1 \leftarrow u_4 \), we can prove that this case could not happen by the similar method.

**Case 4.** There exists a vertex, say \( u_1 \), has three incident edges \( u_1 \leftrightarrow u_2, u_1 \leftrightarrow u_3 \) and \( u_1 \leftrightarrow u_4 \).

Since \( H(u_1,:) \cdot H(u_2,:) = 0 \), we can obtain that \( h_{23} = i, h_{24} = -i \) or \( h_{23} = -i, h_{24} = i \), that is \( u_2 \rightarrow u_3, u_2 \leftarrow u_4 \) or \( u_2 \leftarrow u_3, u_2 \rightarrow u_4 \). Without loss of generality, assume that \( u_2 \rightarrow u_3, u_2 \leftarrow u_4 \). Similarly, we have \( h_{34} = i \) i.e. \( u_3 \rightarrow u_4 \) by \( H(u_1,:) \cdot H(u_3,:) = 0 \). That is \( u_2 \rightarrow u_3, u_2 \leftarrow u_4 \) and \( u_3 \rightarrow u_4 \); see Fig.3.5.

![Figure 3.5: A 3-regular optimum Hermitian energy mixed graph \( G_3 \).](image)

Now we show that the mixed graph \( G_3 \) drawn in Fig.3.5 is switching equivalent to \( G_1 \) drawn in Fig.3.4(a). Let \( H(G_1) \) and \( H(G_3) \) be the Hermitian-adjacency matrix of \( G_1 \) and \( G_3 \), respectively. Assume that \( D(\theta) := \text{diag}(\theta(u_k)|\theta(u_1) = i, \theta(u_2) = \theta(u_3) = \theta(u_4) = 1) \). Then \( H(G_3) = D(\theta)^{-1}H(G_1)D(\theta) \). Namely \( G_1 \sim G_3 \). Hence, the 3-regular optimum Hermitian energy mixed graph with underlying graph \( K_4 \) (up to switching equivalence) is \( G_1 \) drawn in Fig.3.4(a).

Thus, the proof is complete.

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