3-Regular mixed graphs with optimum Hermitian energy*

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Abstract

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

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

AMS Subject Classification 2010: 05C20, 05C50, 05C90.

1 Introduction

Let G be a simple undirected graph with vertex set $V(G)$ and edge set $E(G)$. For an edge subset $S \subseteq E(G)$, a generalized orientation ϕ of G is to give each edge of S an orientation. Then, G^ϕ is called a mixed graph of G with the generalized orientation ϕ. If $S = E(G)$, then ϕ is an orientation of G and the mixed graph G^ϕ is an oriented graph. If $S = \emptyset$, then G^ϕ 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^ϕ. A mixed graph is called *regular* if its underlying graph

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is a regular graph. Similarly, when we say order, size, degree and so on, we mean that these are the parameters of the underlying graph; unless other stated. For undefined terminology and notation, we refer the reader to [2, 5].

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

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

where i is the unit imaginary number. The spectrum $Sp_H(G^\phi)$ of G^ϕ is defined as the spectrum of $H(G^\phi)$. Since $H(G^\phi)$ is an Hermitian matrix, i.e., $H(G^\phi) = [H(G^\phi)]^* := \overline{[H(G^\phi)]}^T$, the eigenvalues $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$ of $H(G^\phi)$ are all real. In [11], Liu and Li introduced the Hermitian energy of the mixed graph G^ϕ, 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

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

For an oriented graph G^ϕ, Adiga et al. [1] introduced the concept of skew adjacency matrix of G^ϕ, denoted by $S(G^\phi)$, which is defined as $S(G^\phi) = -iH(G^\phi)$. Then, the eigenvalues of $S(G^\phi)$ are $\{-i\lambda_1, -i\lambda_2, \dots, -i\lambda_n\}$. The skew energy of an oriented graph G^ϕ is defined as $\mathcal{E}_S(G^\phi) = \sum_{j=1}^{n} |-i\lambda_j|$ by Adiga et al. in [1]. Thus, $\mathcal{E}_H(G^\phi) = \mathcal{E}_S(G^\phi)$, i.e., the Hermitian energy of an oriented graph is equal to its skew energy. For more details about the skew energy, we refer the reader to a survey [9].

The Hermitian energy can be viewed as a generalization of the graph energy. The concept of the energy of a simple undirected graph was introduced by Gutman in [8], which is related to the total π-electron energy of the molecule represented by that graph. Up to now, the graph energy has been extensively studied. For more details, we refer the reader to a book [10].

In [11], Liu and Li gave a sharp upper bound of the Hermitian energy in terms of the order n and the maximum degree Δ of the mixed graph, 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^ϕ is Δ-regular. For convenience, a mixed graph of order n and maximum degree Δ which satisfies $\mathcal{E}_H(G^\phi) = n\sqrt{\Delta}$ is called an *optimum Hermitian energy mixed graph* in this paper. 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 [11], 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^ϕ on n vertices with $\mathcal{E}_H(G^\phi) = n\sqrt{k}$ for each k, $3 \le k \le n$.*

Liu and Li [11] 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. It is worth mentioning that the same problem has been studied by the researchers for the skew energy of oriented graphs. For more review about this problem, readers may refer to [1, 3, 6, 7, 12] and the references therein.

If G_1^ϕ and G_2^ϕ 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, our main goal is to characterize all 3-regular connected optimum Hermitian energy mixed graphs. Thus, this gives a solution to Problem 1.1 for the case $k = 3$.

2 Preliminaries

In [11], Liu and Li gave a sharp upper bound for the Hermitian energy of a mixed graph and a necessary and sufficient condition for a mixed graph to attain the upper bound.

Lemma 2.1 *(11, part of Theorem 3.2). Let G^ϕ be a mixed graph on n vertices with maximum degree Δ. Then $\mathcal{E}_H(G^\phi) \leqslant n\sqrt{\Delta}$.*

Lemma 2.2 *(11, part of Corollary 3.3). Let H be the Hermitian-adjacency matrix of a mixed graph G^ϕ on n vertices. Then $\mathcal{E}_H(G^\phi) = n\sqrt{\Delta}$ 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^ϕ, where $H(u, :)$ and $H(:, u)$ represent the row vector and column vector corresponding to vertex u in $H(G^\phi)$, respectively.*

Moreover, Liu and Li [11] gave a characterization of the k-regular connected optimum Hermitian energy mixed graphs.

Lemma 2.3 *(11, part of Lemma 3.5). Let G^ϕ be a k-regular connected mixed graph with order n $(n \geq 3)$. Then $\mathcal{E}_H(G^\phi) = n\sqrt{k}$ if and only if for any pair of vertices u and v with distance not more than two in G such that $N(u) \cap N(v) \neq \emptyset$ (here and in what follows, $N(x)$ denotes the neighborhood of a vertex x in G), there are edge-disjoint mixed 4-cycles $uxvy$ of the following three types; see Fig.2.1.*

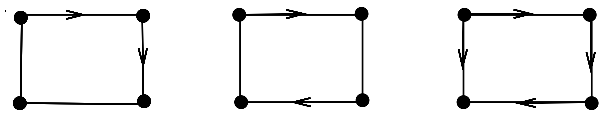

Figure 2.1: Three types of mixed 4-cycles.

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

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

Next we introduce the definition of switching equivalence. Let G^{ϕ} be a mixed graph with vertex set V. The switching function of G^{ϕ} is a function $\theta : V \to \mathrm{T}$, where $\mathrm{T} = \{1, -1\}$. The switching matrix of G^{ϕ} is a diagonal matrix $D(\theta) := diag(\theta(v_k) : v_k \in V)$, where θ is a switching function. Let G^{ϕ_1}, G^{ϕ_2} and G^{ϕ_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 that G^{ϕ_1} and G^{ϕ_2} are switching equivalent, denoted by $G^{\phi_1} \sim G^{\phi_2}$. If two mixed graphs G^{ϕ_1} and G^{ϕ_2} are switching equivalent, then $Sp_H(G^{\phi_1}) = Sp_H(G^{\phi_2})$, which implies that $\mathcal{E}_H(G^{\phi_1}) = \mathcal{E}_H(G^{\phi_2})$. Besides, the number of arcs (or undirected edges) in G^{ϕ_1} is equal to that in G^{ϕ_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 in [11] also introduced the definition of switching equivalence between mixed graphs. However, T was $\{1, i, -i\}$ in their definition. Besides, our definition coincides with the definition of switching equivalence between oriented graphs which is given in [4] when the mixed graphs are oriented graphs.

Let G^{ϕ} be a k-regular optimum Hermitian energy mixed graph. If G^{ϕ} is an oriented graph, then the Hermitian energy of G^{ϕ} is equal to its skew energy. In [6], Gong and Xu characterized the 3-regular optimum Hermitian energy oriented graphs. Moreover, Chen et al. [3] and Gong et al. [7] independently characterized the 4-regular optimum Hermitian energy oriented graphs. The following lemma is the result about the characterization of 3-regular optimum Hermitian energy oriented graphs in [6].

Lemma 2.5 *[6] Let G^{ϕ} be a 3-regular optimum Hermitian energy oriented graph. Then G^{ϕ} (up to isomorphism) is either D_1 or D_2 shown in Fig.2.2.*

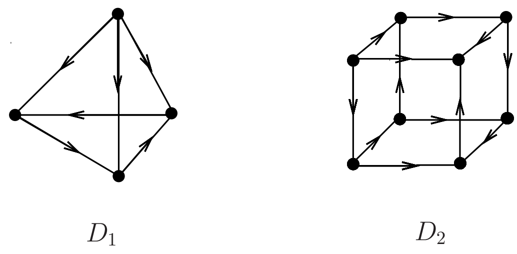

Figure 2.2: 3-regular optimum Hermitian energy oriented graphs.

3 The 3-regular optimum Hermitian energy mixed graphs

In this section, we characterize all 3-regular connected optimum Hermitian energy mixed graphs (up to the switching equivalence defined above).

Let G^{ϕ} be a 3-regular optimum Hermitian energy mixed graph. By Lemma 2.4, it follows that the underlying graph G of G^{ϕ} satisfies that $|N(u) \cap N(v)|$ is even for any two distinct vertices u and v of G. Moreover, from Lemma 3.4 and Theorem 3.5 in [6] we have that if a 3-regular undirected graph G satisfies that $|N(u) \cap N(v)|$ is even for any two distinct vertices u and v of G, then G is either the complete graph K_4 or the hypercube Q_3. Hence, it suffices to consider the 3-regular optimum Hermitian energy mixed graphs with underlying graph K_4 or Q_3.

At first, we consider the case that the underlying graph is the complete graph K_4.

Theorem 3.1 *Let G^{ϕ} be a 3-regular optimum Hermitian energy mixed graph. If the underlying graph G is K_4, then G^{ϕ} is either D_1 shown in Fig.2.2 or G_1 shown in Fig.3.3.*

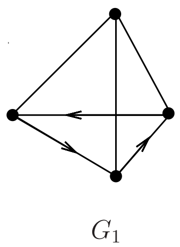

Figure 3.3: Optimum Hermitian energy mixed graph with underlying graph K_4.

Proof. We divide our discussion into four cases:

Case 1. G^{ϕ} is an oriented graph.

From Lemma 2.5, we obtain that G^{ϕ} is D_1 shown in Fig.2.2.

Case 2. G^{ϕ} 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. $u_1 \to u_3$ and $u_1 \to u_4$.

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

Subcase 2.3. $u_1 \to u_3,\ u_1 \leftarrow u_4$ or $u_1 \leftarrow u_3,\ u_1 \to u_4$.

Without loss of generality, assume that $u_1 \to u_3$ and $u_1 \leftarrow u_4$. 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 $u_1 \to u_4$ or $u_1 \leftarrow u_4$. Suppose we have $u_1 \to u_4$. By Lemma 2.2, we have that $H(u_1,:) \cdot H(u_2,:) = 0$. Then, $\overline{h}_{11}h_{21} + \overline{h}_{12}h_{22} + \overline{h}_{13}h_{23} + \overline{h}_{14}h_{24} = h_{23} - ih_{24} = 0$. 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 $u_2 \to u_3, u_2 \leftrightarrow u_4$. If $u_2 \leftrightarrow u_3, u_2 \leftarrow u_4$, then $H(u_1,:) \cdot H(u_3,:) = 0$ from Lemma 2.2. This implies that $\overline{h}_{11}h_{31} + \overline{h}_{12}h_{32} + \overline{h}_{13}h_{33} + \overline{h}_{14}h_{34} = 1 - ih_{34} = 0$. Thus, $h_{34} = -i$, i.e., $u_3 \leftarrow u_4$. However, $H(u_1,:) \cdot H(u_4,:) = \overline{h}_{11}h_{41} + \overline{h}_{12}h_{42} + \overline{h}_{13}h_{43} + \overline{h}_{14}h_{44} = i + i \neq 0$, a contradiction. If $u_2 \to u_3, u_2 \leftrightarrow u_4$, then $H(u_1,:) \cdot H(u_3,:) = 0$ from Lemma 2.2. This implies that $\overline{h}_{11}h_{31} + \overline{h}_{12}h_{32} + \overline{h}_{13}h_{33} + \overline{h}_{14}h_{34} = -i - ih_{34} = 0$. Thus, $h_{34} = -1$, a contradiction.

For the case $u_1 \leftarrow u_4$, we can prove that this could not happen similarly.

Case 4. There exists a vertex, say u_1, having 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, $u_2 \to u_3, u_2 \leftarrow u_4$ or $u_2 \leftarrow u_3, u_2 \to u_4$. Without loss of generality, assume that $u_2 \to u_3, u_2 \leftarrow u_4$. Similarly, we have $h_{34} = i$, i.e., $u_3 \to u_4$ by $H(u_1,:) \cdot H(u_3,:) = 0$. That is, $u_2 \to u_3, u_2 \leftarrow u_4$ and $u_3 \to u_4$; see G_1 shown in Fig.3.3.

The proof is thus complete. ∎

Next, we determine all optimum Hermitian energy mixed graphs with underlying graph Q_3.

Theorem 3.2 *Let G^{ϕ} be a 3-regular optimum Hermitian energy mixed graph. If the underlying graph G is Q_3, then G^{ϕ} (up to switching equivalence) is one of the following graphs: D_2 or H_i, where $i = 1, 2, ..., 6$; see Figs.2.2 and 3.4.*

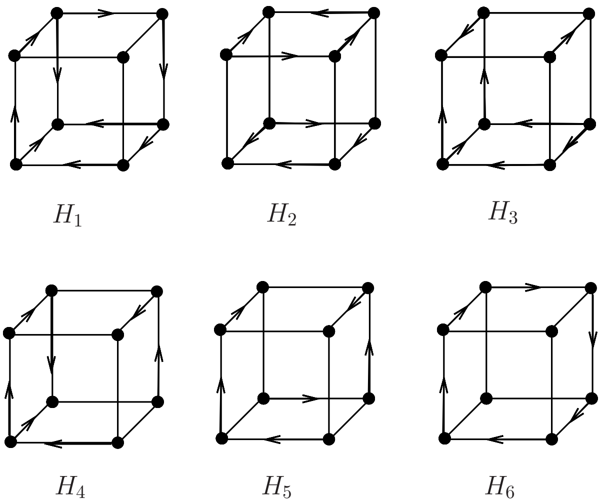

Figure 3.4: Optimum Hermitian energy mixed graphs with underlying graph Q_3.

Proof. We divide our discussion into two cases:

Case 1. G^{ϕ} is an oriented graph.

From Lemma 2.5, we obtain that G^{ϕ} is D_2 shown in Fig.2.2.

Case 2. G^{ϕ} is not an oriented graph. In the following, we replace G^{ϕ} with Q_3^{ϕ} for convenience and assume that $V(Q_3) = \{v_1, v_2, ..., v_8\}$, see Fig.3.5.

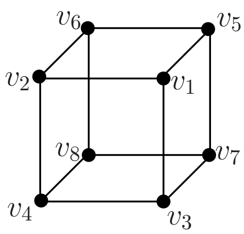

Figure 3.5: Q_3.

Let a (resp., b) denote the number of arcs (resp., undirected edges) in Q_3^{ϕ}, where $a + b = 12$. Since Q_3^{ϕ} is not an oriented graph, we get that $a \leq 11$. Furthermore, there are exactly six mixed 4-cycles in Q_3^{ϕ}. Let C_1, C_2, C_3, C_4, C_5 and C_6 denote the mixed 4-cycle induced by the vertex subset $\{v_1, v_2, v_4, v_3\}$, $\{v_2, v_4, v_8, v_6\}$, $\{v_5, v_6, v_8, v_7\}$, $\{v_1, v_3, v_7, v_5\}$, $\{v_1, v_2, v_6, v_5\}$ and $\{v_3, v_4, v_8, v_7\}$, respectively. By Lemma 2.3, we can deduce that every mixed 4-cycle in Q_3^{ϕ} is one of the three types in Fig.2.1. Thus, we obtain the following claim.

Claim 1: In Q_3^ϕ, every mixed 4-cycle has either two arcs and two undirected edges or four arcs.

It follows that each mixed 4-cycle in Q_3^ϕ has at least two arcs. Then, we have $a \geq \frac{2\times 6}{2} = 6$. Moreover, we can check that $a \neq 10, 11$. Consequently, $6 \leq a \leq 9$. Now we divide the discussion about the values of a and b into four subcases:

Subcase 2.1. $a = 9$, $b = 3$.

In this subcase, we want to determine three undirected edges in Q_3^ϕ. Without loss of generality, suppose $v_1 \leftrightarrow v_3$. By Claim 1, both mixed 4-cycles C_1 and C_4 have two undirected edges and hence we get the following four cases (up to isomorphism) by considering the other two undirected edges in C_1 and C_4.

(1) The other two undirected edges are $v_2 \leftrightarrow v_4$ in C_1 and $v_5 \leftrightarrow v_7$ in C_4. Then, there are three arcs in the mixed 4-cycles C_2 and C_3, which contradicts Claim 1.

(2) The other two undirected edges are $v_1 \leftrightarrow v_2$ in C_1 and $v_5 \leftrightarrow v_7$ in C_4. Then, there are three arcs in the mixed 4-cycles C_5 and C_3, which contradicts Claim 1.

(3) The other two undirected edges are $v_1 \leftrightarrow v_2$ in C_1 and $v_3 \leftrightarrow v_7$ in C_4. Then, there are three arcs in the mixed 4-cycles C_5 and C_6, which contradicts Claim 1.

(4) The other two undirected edges are $v_1 \leftrightarrow v_2$ in C_1 and $v_1 \leftrightarrow v_5$ in C_4. Then, the mixed 4-cycles C_1, C_4 and C_5 should be the first type in Fig.2.1; the mixed 4-cycles C_2, C_3 and C_6 should be the third type in Fig.2.1. Hence, there are two arcs $v_3 \rightarrow v_4, v_4 \rightarrow v_2$ or $v_2 \rightarrow v_4, v_4 \rightarrow v_3$ in C_1, $v_5 \rightarrow v_7, v_7 \rightarrow v_3$ or $v_3 \rightarrow v_7, v_7 \rightarrow v_5$ in C_4, and $v_2 \rightarrow v_6, v_6 \rightarrow v_5$ or $v_5 \rightarrow v_6, v_6 \rightarrow v_2$ in C_5. If there are two arcs $v_3 \rightarrow v_4$ and $v_4 \rightarrow v_2$ in a mixed graph, then we reverse every arc which is incident to vertex v_4 and obtain a new mixed graph denoted by $Q_3^{\phi'}$. Let $D(\theta) = diag(\theta(v_k)|\theta(v_4) = -1 \; and \; \theta(v_k) = 1 \; for \; v_k \in V(Q_3)\backslash\{v_4\})$ (i.e., $D(\theta) = diag(1, 1, 1, -1, 1, 1, 1, 1)$). Then, it follows that $H(Q_3^{\phi'}) = D(\theta)^{-1}H(Q_3^\phi)D(\theta)$. Hence, $Q_3^{\phi'}$ and Q_3^ϕ are switching equivalent by the definition of switching equivalence. Without loss of generality, assume that $v_3 \rightarrow v_4, v_4 \rightarrow v_2$. By a similar discussion, we assume that $v_2 \rightarrow v_6, v_6 \rightarrow v_5$ and $v_5 \rightarrow v_7, v_7 \rightarrow v_3$. Afterwards, we have either $v_4 \rightarrow v_8, v_6 \rightarrow v_8$ or $v_8 \rightarrow v_6, v_8 \rightarrow v_4$ in C_2. Analogously, by switching equivalence we assume that $v_4 \rightarrow v_8, v_6 \rightarrow v_8$ and then $v_7 \rightarrow v_8$. Therefore, we get the graph (up to switching equivalence) H_1 in Fig.3.4.

Subcase 2.2. $a = 8$, $b = 4$.

Now we want to determine four undirected edges in Q_3^ϕ. Based on the discussion of Subcase 2.1, we just need to find one more undirected edge.

If the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_2 \leftrightarrow v_4$ and $v_5 \leftrightarrow v_7$, then there are two undirected edges in C_1 and C_4. Thus, the fourth undirected edge cannot be $v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_4, v_1 \leftrightarrow v_5$ or $v_3 \leftrightarrow v_7$. If the fourth undirected edge is $v_2 \leftrightarrow v_6, v_5 \leftrightarrow v_6, v_4 \leftrightarrow v_8$ or $v_7 \leftrightarrow v_8$, then the resulting graphs are isomorphic. Without loss of generality, suppose

$v_2 \leftrightarrow v_6$. Nevertheless, there are three arcs in C_5, which contradicts Claim 1. If the fourth undirected edge is $v_6 \leftrightarrow v_8$, then the mixed 4-cycles C_5 and C_6 should be the third type in Fig.2.1 and the others should be the second type in Fig.2.1. Thus, we get H_2 (up to isomorphism) in Fig.3.4.

If the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2$ and $v_5 \leftrightarrow v_7$, then there are two undirected edges in C_1 and C_4. Thus, the fourth undirected edge cannot be $v_2 \leftrightarrow v_4, v_3 \leftrightarrow v_4, v_1 \leftrightarrow v_5$ or $v_3 \leftrightarrow v_7$. If the fourth undirected edge is $v_2 \leftrightarrow v_6$, then there are three arcs in C_2, which contradicts Claim 1. By a similar way, we deduce that the fourth undirected edge cannot be $v_6 \leftrightarrow v_8, v_4 \leftrightarrow v_8$ or $v_7 \leftrightarrow v_8$. If the fourth undirected edge is $v_5 \leftrightarrow v_6$, then the mixed 4-cycles C_1 and C_3 should be the first type in Fig.2.1; the mixed 4-cycles C_4 and C_5 should be the second type in Fig.2.1; the mixed 4-cycles C_2 and C_6 should be the third type in Fig.2.1. Hence, there are two arcs $v_3 \rightarrow v_4, v_4 \rightarrow v_2$ or $v_2 \rightarrow v_4, v_4 \rightarrow v_3$ in C_1, and $v_7 \rightarrow v_8, v_8 \rightarrow v_6$ or $v_6 \rightarrow v_8, v_8 \rightarrow v_7$ in C_3. If there are two arcs $v_3 \rightarrow v_4$ and $v_4 \rightarrow v_2$ in a mixed graph, then we reverse every arc which is incident to vertex v_4 and obtain a new mixed graph. By the definition of switching equivalence, we can find the switching matrix $D(\theta) = diag(1, 1, 1, -1, 1, 1, 1, 1)$ to prove that the two mixed graphs are switching equivalent. Without loss of generality, assume that $v_3 \rightarrow v_4, v_4 \rightarrow v_2$. By a similar discussion, we assume that $v_7 \rightarrow v_8, v_8 \rightarrow v_6$. Afterwards, we have either $v_4 \rightarrow v_8$ or $v_8 \rightarrow v_4$. If there is an arc $v_4 \rightarrow v_8$, then we get the other arcs $v_6 \rightarrow v_2, v_1 \rightarrow v_5, v_7 \rightarrow v_3$. Thus, we obtain H_3 depicted in Fig.3.4. If there is an arc $v_8 \rightarrow v_4$, then we get the other arcs $v_2 \rightarrow v_6$, $v_5 \rightarrow v_1$, $v_3 \rightarrow v_7$ and the resulting mixed graph is isomorphic to H_3.

If the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2$ and $v_3 \leftrightarrow v_7$, then there are two undirected edges in C_1 and C_4. Thus, the fourth undirected edge cannot be $v_2 \leftrightarrow v_4, v_3 \leftrightarrow v_4, v_1 \leftrightarrow v_5$ or $v_5 \leftrightarrow v_7$. If the fourth undirected edge is $v_2 \leftrightarrow v_6$, then there are three arcs in C_2, which contradicts Claim 1. By a similar way, we deduce that the fourth undirected edge cannot be $v_5 \leftrightarrow v_6, v_6 \leftrightarrow v_8, v_4 \leftrightarrow v_8$ or $v_7 \leftrightarrow v_8$. Thus, this case could not happen.

If the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2$ and $v_1 \leftrightarrow v_5$, then there are two undirected edges in C_1, C_4 and C_5. Thus, the fourth undirected edge cannot be $v_2 \leftrightarrow v_4, v_3 \leftrightarrow v_4, v_3 \leftrightarrow v_7, v_5 \leftrightarrow v_7, v_2 \leftrightarrow v_6$ or $v_5 \leftrightarrow v_6$. If the fourth undirected edge is $v_4 \leftrightarrow v_8$, then there are three arcs in C_2, which contradicts Claim 1. By a similar way, we deduce that the fourth undirected edge cannot be $v_6 \leftrightarrow v_8$ or $v_7 \leftrightarrow v_8$. Thus, this case could not happen.

Subcase 2.3. $a = 7$, $b = 5$.

Similarly, in order to determine five undirected edges in Q_3^{ϕ}, we just need to find two more undirected edges based on the discussion of Subcase 2.1.

If the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_2 \leftrightarrow v_4$ and $v_5 \leftrightarrow v_7$, then there are two undirected edges in C_1 and C_4. Thus, the other two undirected edges cannot be $v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_4, v_1 \leftrightarrow v_5$ or $v_3 \leftrightarrow v_7$. If one of the other two undirected edges is $v_6 \leftrightarrow v_8$, then there are two undirected edges in C_2 and C_3. By Claim 1, the last undirected edge cannot be $v_2 \leftrightarrow v_6, v_4 \leftrightarrow v_8, v_5 \leftrightarrow v_6$ or $v_7 \leftrightarrow v_8$. Then, there do not exist five undirected edges and hence this case could not happen. If there is an arc between v_6 and v_8, then the other two undirected edges (up to isomorphism) can be $v_2 \leftrightarrow v_6$ and $v_4 \leftrightarrow v_8$, $v_2 \leftrightarrow v_6$ and $v_5 \leftrightarrow v_6$, or $v_2 \leftrightarrow v_6$ and $v_7 \leftrightarrow v_8$. If the other two undirected edges are $v_2 \leftrightarrow v_6$ and $v_4 \leftrightarrow v_8$, then there are three undirected edges in C_2, which contradicts Claim 1. By a similar way, we deduce that the other two undirected edges cannot be $v_2 \leftrightarrow v_6$ and $v_7 \leftrightarrow v_8$. Therefore, the five undirected edges in Q_3^ϕ can be $v_1 \leftrightarrow v_3, v_2 \leftrightarrow v_4, v_5 \leftrightarrow v_7, v_2 \leftrightarrow v_6$ and $v_5 \leftrightarrow v_6$.

By a similar discussion, if the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2$ and $v_5 \leftrightarrow v_7$, then we deduce that the five undirected edges in Q_3^ϕ can be $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_5 \leftrightarrow v_7, v_2 \leftrightarrow v_6$ and $v_6 \leftrightarrow v_8$; if the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2$ and $v_3 \leftrightarrow v_7$, then we deduce that the five undirected edges in Q_3^ϕ can be either $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_7, v_2 \leftrightarrow v_6, v_4 \leftrightarrow v_8$ or $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_7, v_5 \leftrightarrow v_6, v_7 \leftrightarrow v_8$; if the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2$ and $v_1 \leftrightarrow v_5$, then this case could not happen. Regardless of the labels of vertices, the cases of the five undirected edges which we have determined are the same.

Without loss of generality, suppose that the five undirected edges are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_7, v_5 \leftrightarrow v_6$ and $v_7 \leftrightarrow v_8$. Then, the mixed 4-cycles C_1, C_4 and C_6 should be the first type in Fig.2.1; the mixed 4-cycles C_5 and C_3 should be the second type in Fig.2.1; the mixed 4-cycle C_2 should be the third type in Fig.2.1. Hence, there are two arcs either $v_3 \to v_4, v_4 \to v_2$ or $v_2 \to v_4, v_4 \to v_3$ in C_1. If there are two arcs $v_3 \to v_4$ and $v_4 \to v_2$ in C_1, then we have an arc $v_4 \to v_8$ in C_6. Otherwise, there is an arc $v_8 \to v_4$. If there are three arcs $v_3 \to v_4, v_4 \to v_2$ and $v_4 \to v_8$ in a mixed graph, then we reverse every arc which is incident to vertex v_4 and obtain a new mixed graph. Using the switching matrix $D(\theta) = diag(1, 1, 1, -1, 1, 1, 1, 1)$, we can prove that the two mixed graphs are switching equivalent. Without loss of generality, assume that $v_3 \to v_4, v_4 \to v_2$ and $v_4 \to v_8$. Afterwards, we have arcs either $v_7 \to v_5, v_5 \to v_1$ or $v_1 \to v_5, v_5 \to v_7$ in C_4. If there are two arcs $v_7 \to v_5$ and $v_5 \to v_1$ in C_4, then the other arcs are $v_2 \to v_6$ and $v_6 \to v_8$. Thus, we obtain H_4 shown in Fig.3.4. If there are two arcs $v_1 \to v_5$ and $v_5 \to v_7$ in C_4, then the other arcs are $v_8 \to v_6, v_6 \to v_2$ and the resulting mixed graph is isomorphic to H_4.

Subcase 2.4. $a = 6$, $b = 6$.

In order to determine six undirected edges in Q_3^ϕ, we just need to find three more undirected edges based on the discussion of Subcase 2.1.

If the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_2 \leftrightarrow v_4$ and $v_5 \leftrightarrow v_7$, then there are two undirected edges in C_1 and C_4. Thus, the other three undirected edges cannot be $v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_4, v_1 \leftrightarrow v_5$ or $v_3 \leftrightarrow v_7$. If one of the other three undirected edges is $v_2 \leftrightarrow v_6$, then there must have an undirected edge $v_5 \leftrightarrow v_6$ in C_5 by Claim 1. However, the last undirected edge cannot be $v_6 \leftrightarrow v_8, v_4 \leftrightarrow v_8$ or $v_7 \leftrightarrow v_8$ by Claim 1. Then, there do not exist six undirected edges. Similarly, we can show that one of the other three undirected edges cannot be $v_5 \leftrightarrow v_6, v_4 \leftrightarrow v_8$ or $v_7 \leftrightarrow v_8$. Hence, this case could not happen.

By a similar discussion, if the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2$ and $v_5 \leftrightarrow v_7$, then we deduce that the six undirected edges in Q_3^ϕ can be $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_5 \leftrightarrow v_7, v_2 \leftrightarrow v_6, v_4 \leftrightarrow v_8$ and $v_7 \leftrightarrow v_8$; if the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2$ and $v_3 \leftrightarrow v_7$, then we deduce that the six undirected edges in Q_3^ϕ can be either $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_7, v_2 \leftrightarrow v_6, v_6 \leftrightarrow v_8, v_7 \leftrightarrow v_8$ or $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_7, v_5 \leftrightarrow v_6, v_6 \leftrightarrow v_8, v_4 \leftrightarrow v_8$; if the three undirected edges which we have determined are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2$ and $v_1 \leftrightarrow v_5$, then we deduce that the six undirected edges in Q_3^ϕ can be $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_1 \leftrightarrow v_5, v_6 \leftrightarrow v_8, v_4 \leftrightarrow v_8$ and $v_7 \leftrightarrow v_8$. Regardless of the labels of vertices, the case that $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_5 \leftrightarrow v_7, v_2 \leftrightarrow v_6, v_4 \leftrightarrow v_8, v_7 \leftrightarrow v_8$ is the same as the case that $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_7, v_5 \leftrightarrow v_6, v_6 \leftrightarrow v_8, v_4 \leftrightarrow v_8$. Thus, we get the following three cases.

(1) The six undirected edges are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_7, v_2 \leftrightarrow v_6, v_6 \leftrightarrow v_8$ and $v_7 \leftrightarrow v_8$. Then, every mixed 4-cycle in Q_3^ϕ should be the first type in Fig.2.1. Hence, there are two arcs either $v_3 \rightarrow v_4, v_4 \rightarrow v_2$ or $v_2 \rightarrow v_4, v_4 \rightarrow v_3$ in C_1. If there are two arcs $v_3 \rightarrow v_4$ and $v_4 \rightarrow v_2$ in C_1, then we get an arc $v_4 \rightarrow v_8$ in C_6 and $v_8 \rightarrow v_4$ in C_2, a contradiction. Analogously, the case that there are two arcs $v_2 \rightarrow v_4$ and $v_4 \rightarrow v_3$ in C_1 could not happen.

(2) The six undirected edges are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_3 \leftrightarrow v_7, v_5 \leftrightarrow v_6, v_6 \leftrightarrow v_8$ and $v_4 \leftrightarrow v_8$. Then, the mixed 4-cycles C_1, C_2, C_3 and C_4 should be the first type in Fig.2.1; the mixed 4-cycles C_5 and C_6 should be the second type in Fig.2.1. Hence, there are two arcs either $v_3 \rightarrow v_4, v_4 \rightarrow v_2$ or $v_2 \rightarrow v_4, v_4 \rightarrow v_3$ in C_1. If there are two arcs $v_3 \rightarrow v_4$ and $v_4 \rightarrow v_2$ in C_1, then we get the other arcs $v_2 \rightarrow v_6, v_5 \rightarrow v_1, v_7 \rightarrow v_5$ and $v_8 \rightarrow v_7$. Thus, we obtain H_5 shown in Fig.3.4. If there are two arcs $v_2 \rightarrow v_4$ and $v_4 \rightarrow v_3$ in C_1, then we get the other arcs $v_6 \rightarrow v_2, v_1 \rightarrow v_5, v_5 \rightarrow v_7$, $v_7 \rightarrow v_8$ and the resulting mixed graph is isomorphic to H_5.

(3) The six undirected edges are $v_1 \leftrightarrow v_3, v_1 \leftrightarrow v_2, v_1 \leftrightarrow v_5, v_6 \leftrightarrow v_8, v_4 \leftrightarrow v_8$ and $v_7 \leftrightarrow v_8$. Then, every mixed 4-cycle in Q_3^ϕ should be the first type in Fig.2.1. Hence, there are two arcs either $v_3 \rightarrow v_4, v_4 \rightarrow v_2$ or $v_2 \rightarrow v_4, v_4 \rightarrow v_3$ in C_1. If there are two arcs $v_3 \rightarrow v_4$ and $v_4 \rightarrow v_2$ in C_1, then we get the other arcs $v_2 \rightarrow v_6, v_6 \rightarrow v_5, v_5 \rightarrow v_7$ and $v_7 \rightarrow v_3$. Thus, we obtain H_6 shown in Fig.3.4. If there are two arcs $v_2 \rightarrow v_4$ and $v_4 \rightarrow v_3$ in C_1, then we get the other arcs $v_6 \rightarrow v_2, v_5 \rightarrow v_6, v_7 \rightarrow v_5, v_3 \rightarrow v_7$ and the resulting mixed graph is isomorphic to H_6.

Up to now, the proof is complete. ∎

Finally, we summarize all results above as the following theorem, which solve Problem 1.1 for the case $k = 3$.

Theorem 3.3 *Let G^ϕ be a 3-regular mixed graph. Then G^ϕ has optimum Hermitian energy if and only if G^ϕ (up to switching equivalence) is one of the following graphs: D_1, D_2, G_1 or H_i, where $i = 1, 2, ..., 6$; see Figs. 2.2, 3.3 and 3.4.*

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References

[1] C. Adiga, R. Balakrishnan, Wasin So, The skew energy of a digraph, Linear Algebra Appl. 432(2010), 1825–1835.

[2] J. Bondy, U. Murty, Graph Theory, Springer, New York, 2008.

[3] X. Chen, X. Li, H. Lian, 4-Regular oriented graphs with optimum skew energy, Linear Algebra Appl. 439(10)(2013), 2948–2960.

[4] D. Cui, Y. Hou, On the skew spectra of Cartesian products of graphs, Electron. J. Combin. 20(2013), #P19.

[5] D. Cvetković, P. Rowlinson, S. Simić, An Introduction to the Theory of Graph Spectra, London Mathematical Society Student Texts, vol. 75, Cambridge University Press, Cambridge, 2010.

[6] S. Gong, G. Xu, 3-Regular digraphs with optimum skew energy, Linear Algebra Appl. 436(2012), 465–471.

[7] S. Gong, G. Xu, W. Zhong, 4-regular oriented graphs with optimum skew energies, European J. Combin. 36(2014), 77–85.

[8] I. Gutman, The energy of a graph, Ber. Math. Statist. Sekt. Forschungsz. Graz 103(1978), 1-22.

[9] X. Li, H. Lian, Skew energy of oriented graphs, Chapter 8 in "I. Gutman, X. Li (Eds.), Energies of Graphs- Theory and Applications", Mathematical Chemistry Monograph No.17, 2016, pp.191–236.

[10] X. Li, Y. Shi, I. Gutman, Graph Energy, Springer, New York, 2012.

[11] J. Liu, X. Li, Hermitian-adjacency matrices and Hermitian energies of mixed graphs, Linear Algebra Appl. 466(2015), 182–207.

[12] G. Tian, On the skew energy of orientations of hypercubes, Linear Algebra Appl. 435(2011), 2140-2149.