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When a Polyhex is Kekuléan

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Abstract: The term "polyhex" is used to denote benzenoids and coronoids together. Benzenoids are polyhexes without holes, while coronoids are polyhexes with one or more holes. Kekuléan polyhexes are polyhexes with at least one Kekulé structure. A uniform criterion is given for the first time to recognize Kekuléan polyhexes.

1 Introduction

A benzenoid [1], also called benzenoid system, is a finite 2-connected plane graph in which every interior face is bounded by a regular hexagon of side length 1. A coronoid [2] can be regarded as a sort of benzenoid with holes. A coronoid G can be obtained from a benzenoid B by deleting all the vertices and edges in the interior of a group of pairwise disjoint cycles $C_1, C_2, \cdots, C_m (m \geq 1)$ which are inside B, i.e. C_i contains no vertex on the perimeter of B. Besides, each C_i must have size greater than 6. These cycles are called the inner perimeters of G, while the perimeter C_0 of B is called the outer perimeter of G. If G has exactly one inner perimeter, G is called a single coronoid ; otherwise, G is called a multiple coronoid. A coronoid is either a single coronoid or a multiple coronoid. A coronoid G and the benzenoid B from which G is obtained are given in Fig.1.

The term "polyhex" is used to denote benzenoids and coronoids together. Thus benzenoids are polyhexes without holes, while coronoids are polyhexes with one or more holes.

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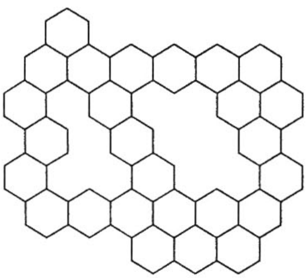
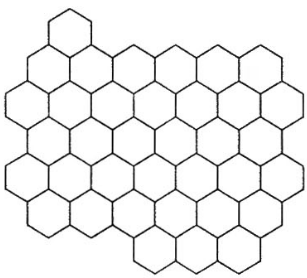
Polyhexes are of great chemical relevance[1,2]. Research in this area has attracted the constant attention of both chemists and mathematicians. The so-called perfect matching, or 1-factor of a polyhex corresponds to the notion of Kekulé structure from physical chemistry. The importance of Kekulé structure is generally recognized in theoretical chemistry. I n particular, the number of Kekulé structures is quantitatively correlated with several basic physico-chemical properties of polyhexes: thermodynamic stability, aromaticity, reactivity, etc [3].



G



B

Fig.1

Since a polyhex is the skeleton of some aromatic hydrocarbon molecule if and only if it has a Kekulé structure, the problem of determining whether or not a given polyhex has a Kekulé structure is of some significance in the study of the topological properties of polyhexes. For benzenoids, many criteria and methods have been given to recognize Kekuléan benzenoids (see [4] and the references cited therein, [7-10]). For coronoids , only a necessary and sufficient condition was given for single coronoids to have a Kekulé structure [5]. No simple criterion is reported for a multiple coronoid to have a Kekulé structure. In this paper we intend to fill this gap , and give a simple uniform criterion for a polyhex to be Kekuléan, whether it is a benzenoid , or a single coronoid, or a multiple coronoid.

2 Some definitions

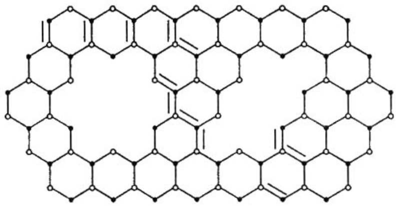
Let G be a polyhex with perimeters $C_0, C_1, \cdots, C_m$, where C_0 is the outer perimeter, and C_i is the inner perimeter (if any) for $i = 1, \cdots, m$. let E be a subset of the edge set of G. $G - E$ is the subgraph of G obtained by deleting all the edges of E. E is said to be an edge-cut of G if $G - E$ is disconnected.

From the definitions of polyhexes, it is easy to see that they are bipartite graphs. Thus they are 2-colorable. In the following, we make the convention that the vertices of a polyhex in question have been colored black and white so that the end vertices of any edge have different colors. By $B(G)$ and $W(G)$ we denote the set of black vertices of G and the set of white vertices of G, respectively.

Definition 1[6] Let G be a polyhex. An edge-cut E is called an elementary edge-cut if

it satisfies the following two statements:
1. $G - E$ has exactly two components;
2. the end vertices of the edges of E have the same color when they lie in the same component of $G - E$.

In Fig.2 an elementary edge-cut E (the edges of E are indicated by double lines.) and the two components of $G - E$: $G_1(E)$ and $G_2(E)$ are given.



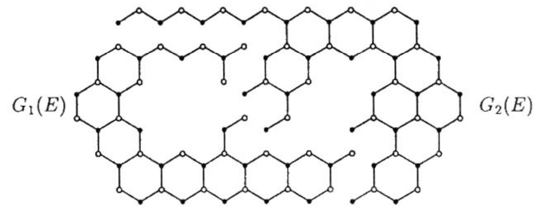


Fig.2

Definition 2 [5] A straight line segment P_1P_2 is called a cut segment from C_i to C_j if
1. P_1 is the center of an edge e_1 on C_i and P_2 is the center of an edge e_2 on C_j;
2. P_1P_2 is orthogonal to both e_1 and e_2;
3. any point of P_1P_2 is either an interior or a boundary point of some hexagon of G.

Definition 3 [5] A broken line segment P_1QP_2 is called a generalized cut (g−cut) segment from C_i to C_j if
1. P_1 is the center of an edge e_1 on C_i and P_2 is the center of an edge e_2 on C_j;
2. P_1Q and P_2Q are orthogonal to e_1 and e_2, respectively;
3. Q is the center of a hexagon of G, P_1Q and P_2Q form an angle of $\pi/3$ or $5\pi/3$;
4. any point of P_1QP_2 is either an interior or a boundary point of some hexagon of G.

A special cut segment is either a cut segment or a g−cut segment. A special edge-cut E_{ij} form C_i to C_j is the set of edges of G intersected by a special cut segment form C_i to C_j. A special edge-cut E_{ii} form C_i to C_i is said to be of type I, a special edge-cut E_{ij} form C_i to C_j with $i \neq j$ is said to be of type II.

Definition 4 Let $E = E_{i_1i_2} \cup E_{i_2i_3} \cup \cdots \cup E_{i_ri_1}$, where $E_{i_1i_2}, E_{i_2i_3}, \cdots, E_{i_ri_1}$ are r disjoint special edge-cuts of type II, $E_{i_ji_k}$ corresponds to a special cut segment from C_{i_j} to C_{i_k}, and $i_s \neq i_t$ if $s \neq t$. E is said to be a standard combination of type II if the end vertices of the edges of E have the same color when they lie in the same component of $G-E$.

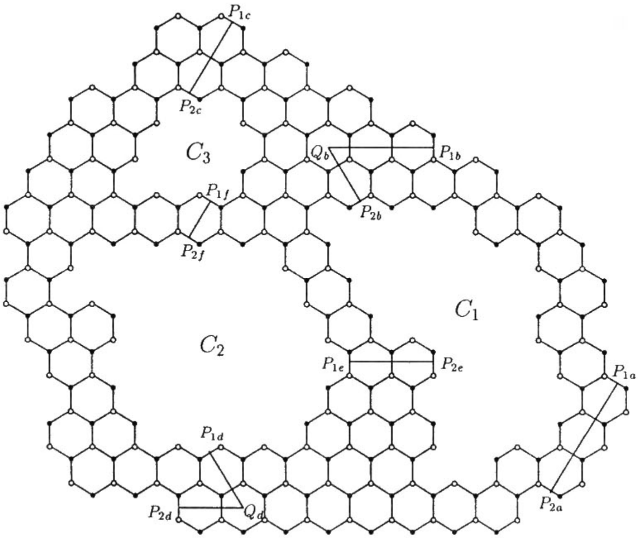


Fig.3

In Fig.3, let E_{01} be the special edge-cut corresponding to the special cut segment $P_{1b}Q_bP_{2b}$, E_{12} the special edge-cut corresponding to the special cut segment $P_{1e}P_{2e}$, E_{20} the special edge-cut corresponding to the special cut segment $P_{1d}Q_dP_{2d}$. Then $E = E_{01} \cup E_{12} \cup E_{20}$ is a standard combination of type II. While the two special edge-cuts corresponding to the special cut segments $P_{1c}P_{2c}$ and $P_{1f}P_{2f}$, respectively, and the special edge-cut corresponding to the special cut segment $P_{1d}Q_dP_{2d}$ do not constitute a standard combination of type II.

Remark 1: It is evident that $G-E$ has exactly two components if E is a special edge-cut of type I, or E is a standard combination of type II; and the end vertices of the edges of E have the same color when they lie in the same component of $G-E$. Thus a special edge-cut of type I , or a standard combination of type II is an elementary edge-cut. But an elementary edge-cut need not be a special edge-cut of type I or a standard combination of type II (cf. Fig.2 and Fig.3)

Suppose that S is a subset of the vertex set $V(G)$ of G.The neighbor set $N(S)$ of S is the set of vertices which are not in S but adjacent to at least one vertex in S. By $\langle S \cup N(S) \rangle$ we denote the induced subgraph of G, i.e. the subgraph of G whose vertex set is $S \cup N(S)$ and whose edge set is the set of those edges of G that have both end vertices in $S \cup N(S)$. Assume that E is an elementary edge-cut. Then it is not difficult to see that the two components of $G - E$, say G_1 and G_2, can be expressed as: $G_1 = \langle X_1 \cup N(X_1)\rangle$ and $G_2 = \langle X_2 \cup N(X_2)\rangle$, where $X_1 \cup N(X_2) = W(G)$ and $X_2 \cup N(X_1) = B(G)$; or $X_1 \cup N(X_2) = B(G)$ and $X_2 \cup N(X_1) = W(G)$. In the case $|B(G)| = |W(G)|$, we have $|N(X_1)| - |X_1| = |N(X_2)| - |X_2|$, and we set $d(E) = |N(X_1)| - |X_1| = |N(X_2)| - |X_2|$.

3 Main result

We formulate our main result as a theorem:

Theorem Let G be a polyhex. Then G is Kekuléan if and only if :

1. $|W(G)| = |B(G)|$;
2. $d(E) \geq 0$ for every special edge-cut E of type I, and for every standard combination E of type II (if any).

The known simple criteria to recognize Kekuléan benzenoids and single coronoids are direct consequences of the above theorem:

Corollary 1:[4] A benzenoid is Kekuléan if and only if :

1. $|W(G)| = |B(G)|$;
2. $d(E) \geq 0$ for every special edge-cut E of type I

Proof. Since a benzenoid is a polyhex without holes, it has no inner perimeter. Hence it has no special edge-cuts of type II, and therefore no standard combination of type II.

Corollary 2: [5] Let G be a single coronoid. Then G is Kekuléan if and only if :

1. $|W(G)| = |B(G)|$;
2. $d(E) \geq 0$ for every special edge-cut E of type I, and for every standard combination E of type II.

Proof: Immediately from the theorem.

4 Lemmas

Before proving of the main theorem, we need some lemmas.

Lemma 1 [11] Let G be a bipartite graph with bipartition (X, Y). Then G has a matching that saturates every vertex in X if and only if $|N(S)| \geq |S|$ for all $S \subseteq X$, where $N(S)$ is the neighbor set of S in G.

Lemma 2 Let G be a Kekuléan polyhex. Then the following conditions hold:

1. $|B(G)| = |W(G)|$;
2. $d(E) \geq 0$ for every special edge-cut of type I and for every standard combination of type II.

Proof. Suppose that G has a Kekulé structure. Since G is a bipartite graph with bipartition $(W(G), B(G))$, condition 1 certainly holds. Let E be a special edge-cut of type I or a standard combination of type II, and let $G_1(E)$ and $G_2(E)$ be the two components of $G - E$. Let $G_1 = \langle X_1 \cup N(X_1)\rangle$, where $X_1 \subseteq B(G)$ or $X_1 \subseteq W(G)$. By Lemma 1, $|N(X_1)| \geq |X_1|$. Hence $d(E) = |N(X_1)| - |X_1| \geq 0$.

Lemma 3[6] Let G be a connected plane bipartite graph each interior vertex of which has the same degree. Then G has a perfect matching if and only if :

1. $|W(G)| = |B(G)|$;
2. $d(E) \geq 0$ for every elementary edge-cut E containing a boundary edge of G.

Remark 2: A boundary edge of G is an edge lying on some boundary of G, an interior vertex of G is a vertex not lying on any boundary of G. Since a polyhex is a bipartite graph, and each interior vertex is of degree three, the above lemma holds for polyhexes.

Let G be a polyhex, E an elementary edge-cut containing a boundary edge. Denote by $G_1(E)$ and $G_2(E)$ the two components of $G - E$. In order to separate $G_1(E)$ from $G_2(E)$, we use a Jordan curve J, i.e. a closed non-self-intersected curve in the plane. Then J intersects each edge in E. We make the convention that J intersects each edge in E at the midpoint of the edge; and if J passes a hexagon of G, it must pass its center; and if J turns within a hexagon of G, it turns at the center of the hexagon. Since E is an elementary edge-cut, the end vertices of the edges in E have the same color when they lie in $G_1(E)$. The same is true for the case when they lie in $G_2(E)$. Hence at each turning point of J the angle is $\pi/3$ or $5\pi/3$.

Suppose that G has no Kekulé structure and condition 1 holds. Then by Lemma 3 there exists an elementary edge-cut E containing a boundary edge such that $d(E) < 0$. Let A denote the set of all such elementary edge-cuts, and let α denote the minimum cardinality of the elementary edge-cuts in A, i.e. $\alpha = \min\{|E| \; |E \in A\}$. Denote by A_α the set of elementary edge-cuts in A each of which has cardinality α, i.e. $A_\alpha = \{E \in A| \; |E| = \alpha\}$. One can see that A_α is a subset of A. For convenience, in the following we may assume , without loss of generality, that $|V(G_1(E))| \geq |V(G_2(E))|$, where $|V(G_i(E))|$ is the cardinality of the vertex set of $G_i(E)$. Denote by V_E the cardinality of $V(G_1(E))$. Let

$$\beta = \max\{V_E \, |E \in A_\alpha\}$$
$$A_{\alpha\beta} = \{E \in A_\alpha| \; V_E = \beta\}$$

Let $E \in A_{\alpha\beta}$. Note that if the corresponding Jordan curve J traverses some perimeter C_i, it must traverses it twice. Now suppose that the edges in E are met by J in the cyclic order: $e_1, e_2, \cdots, e_{p_1}; e_{p_1+1}, \cdots, e_{p_2}; e_{p_2+1}, \cdots\cdots, e_{p_{q-1}}; e_{p_{q-1}+1}, \cdots, e_{p_q}$, where e_{p_i} and e_{p_i+1} are on C_{u_i} for $i = 1, 2, \cdots, q-1$; e_1 and e_{p_q} are on C_{u_q}; e_j is not on any C_t for $t = 1, 2, \cdots, m$; when $j \neq 1, p_1, p_1+1, p_2, p_2+1, \cdots, p_q$.

Since $G_1(E)$ and $G_2(E)$ are both connected, it is obvious that $C_{u_1}, C_{u_2}, \cdots, C_{u_q}$ are pairwise distinct. Let

$$E_r = \{e_{p_{r-1}+1}, e_{p_{r-1}+2}, \cdots, e_{p_r}\} \quad (r = 1, 2, \cdots, q)$$

here we make the convention that $p_0 = 0$. Then $E = E_1 \cup E_2 \cup \cdots \cup E_q$. Denote by J_r the segment of J between the midpoint of $e_{p_{r-1}+1}$ and the midpoint of e_{p_r}.

With the above notation, we have the following lemma.

Lemma 4 If a polyhex G has no Kekulé structure and $|W(G)| = |B(G)|$, then there is an elementary edge-cut $E \in A_{\alpha\beta}$ such that at each turning point of J_r the vertices and the edges within the angle of $\pi/3$ belong to $G_1(E)$.

Proof. As mentioned above, at each turning point of J_r, the angle is either $\pi/3$ or $5\pi/3$. If the lemma is false, then the vertices and and the edges within the angle of $\pi/3$ belong to $G_2(E)$, while those within the angle of $5\pi/3$ belong to $G_1(E)$ (cf. Fig.4). First, suppose that $G_2(E) - \{b_1, w_1\}$ is disconnected, which implies that w_1 is on some of the perimeters $C_{u_1}, C_{u_2}, \cdots, C_{u_q}$, say C_{u_i}. Then $G_2(E) - \{b_1, w_1\}$ has two components: $G_2'(E) = \langle X_2' \cup N(X_2')\rangle$, $G_2''(E) = \langle X_2'' \cup N(X_2'')\rangle$. Let $G_1(E) = \langle X_1 \cup N(X_1)\rangle$, $G_2(E) =$

$\langle X_2 \cup N(X_2)\rangle$. We have:

$$|X_2| = |X_2'| + |X_2''| + 1, |N(X_2)| = |N(X_2')| + |N(X_2'')| + 1$$

Therefore, $|N(X_2)| - |X_2| = |N(X_2')| - |X_2'| + |N(X_2'')| - |X_2''|$. Bear in mind that $E \in A_{\alpha\beta}$. Hence $d(E) = |N(X_2)| - |X_2| < 0$. Thus at least one of "$|N(X_2')| - |X_2'| < 0$" and "$|N(X_2'')| - |X_2''| < 0$" holds. Without loss of generality, we may assume that $|N(X_2'')| - |X_2''| < 0$. Let $E_r' = \{e_{p_{r-1}+1}, e_{p_{r-1}+2}, \cdots, e_s, e_1^*\}$ and $E_r'' = \{f, e_{s+2}, \cdots, e_{p_r}\}$. Since w_1 is on C_{u_i}, then $E^* = E_{i+1} \cup E_{i+2} \cup \cdots \cup E_{r-1} \cup E_r'$ or $E^* = E_r'' \cup E_{r+1} \cup \cdots \cup E_i$ is an edge-cut with some boundary edges. One can check that E^* satisfies the following conditions:

1. the two components of $G - E^*$ are $G_1(E^*) = \langle (X_1 \cup N(X_2') \cup \{b_1\}) \cup (N(X_1) \cup X_2' \cup \{w_1\})\rangle$ and $G_2(E^*) = \langle X_2'' \cup N(X_2'')\rangle$;
2. the end vertices of E^* have the same color when they lie in the same component of $G - E^*$;
3. $d(E^*) = |N(X_2'')| - |X_2''| < 0$;
4. $|E^*| < |E|$.

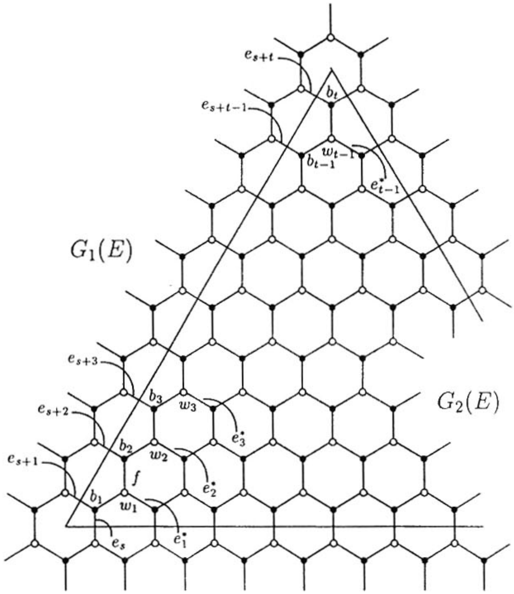


Fig.4

The above conditions 1-3 ensure that E^* is an elementary edge-cut and $E^* \in A$. Condition 4 contradicts that $E \in A_\alpha$, i.e. the cardinality of E is the minimum among all the elementary edge-cuts in A. This contradiction is caused by our assumption that $G_2(E) - \{b_1, w_1\}$ is disconnected. Therefore, $G_2(E) - \{b_1, w_1\}$ is connected. Now let

$E'_r = E_r \cup \{e_1^*, f_1\} - \{e_s, e_{s+1}\}$ (cf. Fig.4), $E' = E_1 \cup E_2 \cup \cdots \cup E_{r-1} \cup E'_r \cup E_{r+1} \cup \cdots \cup E_q$. Then E' is an elementary edge-cut with $|E'| = |E|$. Therefore, $E' \in A_\alpha$. Note that $V(G_1(E')) = V(G_1(E)) \cup \{b_1, w_1\}$. Thus $|V(G_1(E'))| > |V(G_1(E))|$. This contradicts that $E \in A_{\alpha\beta}$, namely, $V(G_1(E))$ has the maximum cardinality among all the elementary edge-cuts of A_α. Consequently, the lemma follows.

5 The proof of the theorem

Necessity follows immediately from Lemma 2.

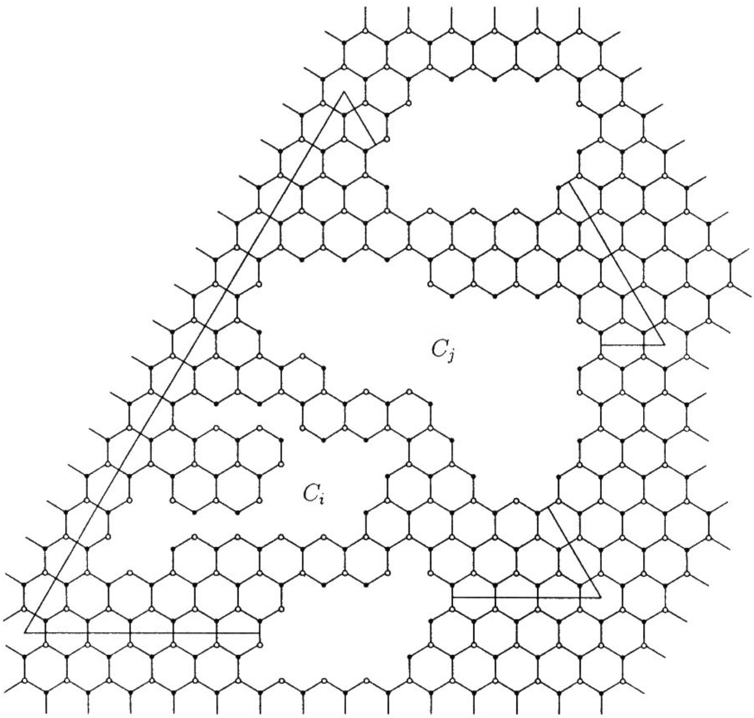


Fig.5

Sufficiency. It suffices to prove that if G has no Kekulé structure and condition 1 holds, then there exists a special edge-cut E of type I or a standard combination E of type

II such that $d(E) < 0$. By the above statement and Lemma 4, there is an elementary edge-cut $E \in A_{\alpha\beta}$ containing at least one boundary edge satisfying: the edges in E are intersected by the corresponding Jordan curve J in cyclic order, and J intersects some perimeters $C_{u_1}, C_{u_2}, \cdots, C_{u_q}$, and J_r (the segment of J between the midpoint of $e_{p_{r-1}+1}$ and the midpoint of e_{p_r}) is a line segment or a broken line segment. In the following we prove that J_r is a special cut segment, and thus E_r is a special edge-cut.

If J_r is already a line segment, there is nothing to prove. Now suppose that J_r is a broken line segment with at least one turning point. By Lemma 4, at each turning point of J_r the vertices and the edges within the angle of $\pi/3$ belong to $G_1(E)$, while those within the angle of $5\pi/3$ belong to $G_2(E)$. If J_r has exactly one turning point, then it is a special cut segment already. Now suppose that J_r has more than one turning point (cf. Fig.5).

Let $E_r' = E_r \cup \{e_1^*, e_2^*, \cdots, e_{t-1}^*\} - \{e_s, e_{s+1}, e_{s+2}, \cdots, e_{s+t}\}$, $E' = E \cup E_r' - E_r = E_1 \cup E_2 \cup \cdots \cup E_{r-1} \cup E_r' \cup E_{r+1} \cup \cdots \cup E_q$. (cf. Fig.4) One can check that $d(E') = d(E) - 1 < d(E) < 0$, $G_1(E') = G_1(E) - \{b_1, b_2, \cdots, b_t; w_1, w_2, \cdots, w_{t-1}\}$ and $G_2(E') = G_2(E) \cup \{b_1, b_2, \cdots, b_t; w_1, w_2, \cdots, w_{t-1}\}$. Evidently, $G_2(E')$ is connected. If $G_1(E')$ is also connected, then $E' \in A$. Note that $|E'| = |E| - 1 < |E|$, which contradicts that the cardinality of E is the minimum among all the edge-cuts in A. Hence $G_1(E)$ is disconnected. This implies that some of the vertices in $\{b_1, b_2, \cdots, b_t; w_1, w_2, \cdots, w_{t-1}\}$ lie on some perimeter of G. There are two possibilities:

Case 1 Vertices $w_i, b_{i+1}, w_{i+1}, b_{i+2}, w_{i+2}, \cdots, b_{i+p}, w_{i+p}$ belong to perimeter $C_j (j \neq u_1, u_2, \cdots, u_q)$, $b_{i+p+1}, w_{i+p+1}, \cdots, b_{i+p+h}$ do not belong to any perimeter of G, $w_{i+p+h}, b_{i+p+h+1}, \cdots, w_{i+p+h+v}$ belong to the same perimeter C_j (cf. Fig.5).

Case 2 Vertices $w_j, b_{j+1}, w_{j+1}, b_{j+2}, w_{j+2}, \cdots, b_{j+a}, w_{j+a}$ belong to perimeter $C_i (i \in \{u_1, u_2, \cdots, u_q\})$(cf. Fig.5).

Note that the above two cases may occur simultaneously. Thus $G_1(E)$ has at least two components.. Then we can find a series of elementary edge-cuts: $E^1, E^2, \cdots, E^t$, each of which is a special edge-cut of type I or a standard combination of type II. We have $\sum_{i=1}^{t} d(E^i) = d(E) - 1 < 0$. Hence at least one of $E^1, E^2, \cdots, E^t$, say E^h, satisfies $d(E^h) < 0$. Therefore, $E^h \in A$. Note that $|E^h| < |E|$(cf.Fig.5), contradicting that $E \in A_\alpha$. Therefore, J_r has at most one turning point, i.e. J_r is a special cut segment. Then the corresponding edge-cut E_r is a special edge-cut. If $q = 1$, then $E = E_1$ is a special edge-cut of type I. If $q > 1$, then $E = E_1 \cup E_2 \cup \cdots \cup E_q$ is a standard combination of type II. The proof is thus completed.

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