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On the existence of multiply connected monolayered cyclofusenes with given parameters

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For a given bipartite graph G its skewness is defined as the difference between the sizes of its classes of bipartition. We show that a multiply connected monolayered cyclofusene with $m \geqslant 2$ internal holes and skewness k exists if and only if $0 \leqslant k \leqslant 2m-2$, thus settling in affirmative two conjectures raised in a recent paper by Karimi et al.

KEY WORDS: multiply connected monolayered cyclofusene, skewness

1. Introduction

A **multiply connected monolayered cyclofusene** (MMC) is a finite subset of the infinite hexagonal lattice that has at least two internal non-hexagonal regions called **holes**. Furthermore, each edge belongs to a hexagon, and each hexagon has two (non-adjacent) edges such that one of them is shared with an internal hole, and the other one either with another internal hole, or with the outer unbounded region. One can think of an MMC as of a continent, surrounded by an ocean (the exterior region), with at least two interior seas (holes), and divided into hexagonal countries in such a way that each country has access to (at least) two different bodies of water. For each MMC we construct its graph G by taking the vertices of hexagons as the vertices of G and the edges of hexagons as the edges of G. So constructed graph is planar and bipartite, since it is a subgraph of the planar and bipartite graph corresponding to the whole lattice. This correspondence enables us to formulate (and solve) problems concerning MMCs using the language of graph theory.

A graph G is **bipartite** if its vertex set $V(G)$ can be partitioned into two classes, B and W, such that each edge e of G has one end in B and the other end in W. We call the vertices from B black, and the vertices from W white. The **skewness** of G is defined as $k(G) = \big||B| - |W|\big|$, where $|B|$ and $|W|$ denote the number of black and white vertices, respectively. If $k(G) = 0$, i.e. $|B| = |W|$, we call the graph G **balanced** or **equitable**.

The problem of equitability of MMC graphs was considered in a recent paper by Karimi et al. [1]. They showed that the problem is equivalent to the problem of equitability of the set S of interior vertices of G, where a vertex is called **interior** if it belongs to three hexagons. Alternatively, a vertex is interior if it does not belong to a non-hexagonal side of G. The authors concluded their paper by stating two conjectures.

Conjecture 1 [1]. Let G be an MMC graph with $m \geqslant 2$ holes. Then $k(G) \leqslant 2m-2$.

Conjecture 2 [1]. For any $m \geqslant 2$ and $0 \leqslant k \leqslant 2m-2$ there exists an MMC graph with m holes and $k(G) = k$.

Conjecture 2 states that $k(G)$ interpolates between 0 and $2m-2$, while Conjecture 1 claims that there are no MMC graphs with m holes and $k(G) > 2m-2$. We will prove both conjectures by establishing the following result.

Theorem 1. An MMC graph with $m \geqslant 2$ holes and skewness k exists if and only if $0 \leqslant k \leqslant 2m-2$.

We first state and prove some auxiliary results.

Lemma 1. Let G is an MMC graph and S the set of its interior vertices. Then the graph $G[S]$ induced by S consists of disjoint union of isolated vertices and edges.

Proof. Let us suppose that a component of $G[S]$ has more than two vertices. Then it must contain either a triangle or a path P_2 on three vertices as a subgraph. The first possibility can be ruled out, since $G[S]$ is bipartite. Hence, it must be P_2. Since all vertices of S are interior, the three vertices of P_2 must all belong to same hexagon A. But then hexagon A must have at least four consecutive edges shared with other hexagons (see figure 1), and the remaining two edges cannot be shared with two different non-hexagonal sides of G. Hence, no component of $G[S]$ contains more than two vertices, and the claim follows. □

Let us denote by $\mathcal{G}_{m,k}$ the set of all MMC graphs with m holes and skewness k. Now theorem 1 can be alternatively formulated.

Theorem $1'$**.** Let $m \geqslant 2$ be a positive integer. Then $\mathcal{G}_{m,k} \neq \emptyset \iff 0 \leqslant k \leqslant 2m-2$.

We proceed by showing that $\mathcal{G}_{m,k}$ are non-empty for small values of k.

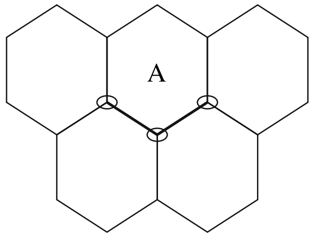


Figure 1. With proof of lemma 1.

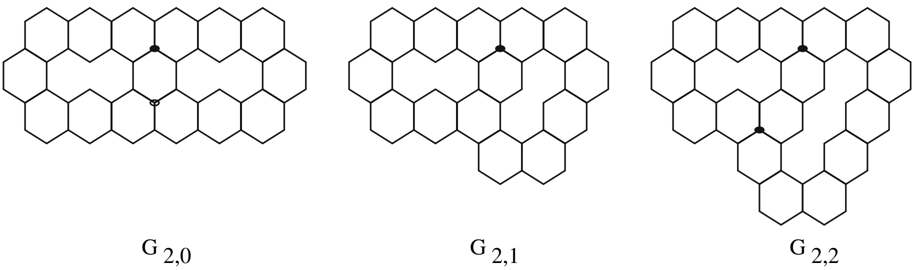


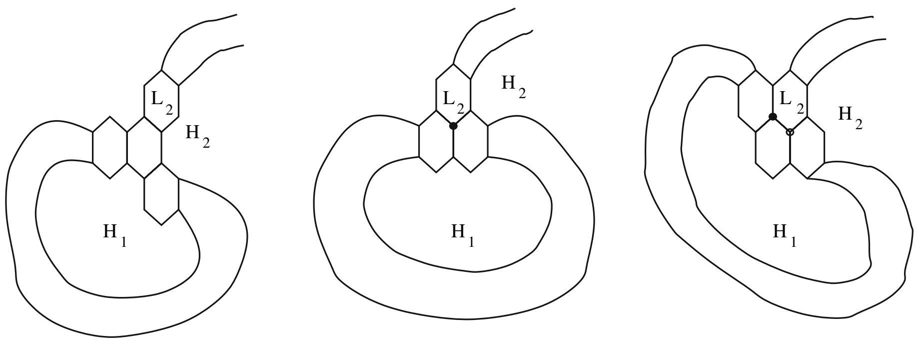
Figure 2. With proof of lemma 2.

Lemma 2. $\mathcal{G}_{2,k} \neq \emptyset$ for $k = 0, 1, 2$.

Proof. The claim follows immediately from figure 2 by noting that $G_{2,k}$ belongs to $\mathcal{G}_{2,k}$ for $k = 0, 1$ and 2. □

Lemma 3. Let G be an MMC graph with $m \geqslant 2$ holes and S the set of its interior vertices. Then the number of isolated vertices in S does not exceed $2m - 2$.

Proof. Let us denote by H_1 one of m holes in G. The graph induced by all hexagons that share an edge with H_1 we denote by G_1. It is obvious that G_1 is a cyclofusene, and hence contains no interior vertices. Let H_2 be a hole of G that shares an edge with a hexagon from G_1. (We know that such a hole exists.) Denote by L_2 the subgraph of G induced by all hexagons sharing an edge with H_2 that are not in G_1. It is clear from the definition of MMC that L_2 is a benzenoid chain, and that its two end-hexagons each share one, two, or three edges with G_1. The three possibilities are shown in figure 3(a)–(c), respectively. (The possibility of sharing four or more edges is ruled out by lemma 1.) Now we set $G_2 = G_1 \cup L_2$, and proceed inductively by adding one benzenoid chain for each hole until we have completed the whole graph G. Obviously, the attachments of types (a) and (c) do not increase the number of isolated vertices in S, and in the worst case, each of $m - 1$ benzenoid chains contributes two isolated vertices to S. □



(a) **(b)** **(c)**

Figure 3. With proof of lemma 3.

Since each isolated edge in $G[S]$ is itself balanced, the skewness of S (and hence of G) cannot exceed the number of isolated vertices in S. Hence, conjecture 1 follows as a corollary of lemma 3. Even more, the upper bound of conjecture 1 is sharp.

Lemma 4. $\mathcal{G}_{m,2m-2} \neq \emptyset$ for all $m \geqslant 2$.

Proof. We start from $G_{2,2}$ and add $m-2$ benzenoid chains in such way that each of them generates two interior vertices of the same color. One way to do it is shown in figure 4. For a given m we start from $G_{2,2}$ and add $m-2$ benzenoid chains consisting of 10, 12, 14, ..., $2m+4$ hexagons. This procedure results in a graph with m holes, m^2+5m+2 hexagons, and skewness $2m-2$. Hence, the class $\mathcal{G}_{m,2m-2}$ is not empty, for all $m \geqslant 2$. □

The procedure of lemma 4 is not the only way to build a graph from $\mathcal{G}_{m,2m-2}$. It might be interesting to determine the minimum number of hexagons necessary for building a graph from $\mathcal{G}_{m,2m-2}$.

It is clear from definition of MMC that no hexagon can share four edges with the exterior region. Among the hexagons sharing three edges with the exterior region there must be some that are in a sense extremal. More precisely, we call a hexagon E of an MMC G **exposed** if a line through its two opposite vertices divides the plane so that one open half-plane contains only two vertices of G. An example is shown in figure 5. By considering the inner dual [2] of the graph induced by all hexagons of G sharing an edge with the exterior region, we obtain a closed curve in hexagonal lattice. Since each exposed hexagon contributes $1/6$ to the winding number of this curve, and since this winding number is equal to one, it follows that an MMC graph has six exposed hexagons.

Let G_1 and G_2 be two MMC graphs with exposed hexagons E_i in G_i, respectively. A **splice** of G_1 and G_2 is defined as the graph obtained by identifying

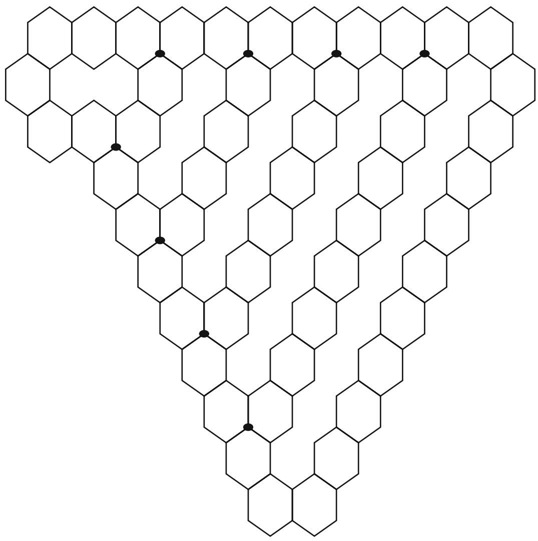


Figure 4. Graph $G_{5,8}$.

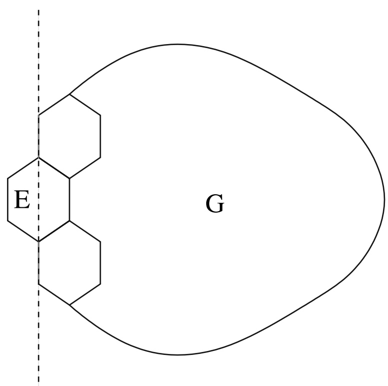


Figure 5. An exposed hexagon.

their exposed hexagons in such a way that no other parts of G_1 and G_2 overlap. A schematic example is shown in figure 6. We denote the splice of G_1 and G_2 by $G_1 \cdot G_2$.

It is obvious from definition that two MMC graphs can be spliced in many ways, since each of them contains six exposed hexagons. No matter how we chose exposed hexagons, a splice of two MMC graphs will always result in another MMC graph. Moreover, the operation is additive with respect to the defining parameters of MMC graphs.

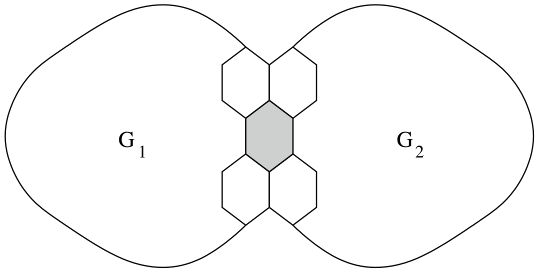


Figure 6. Splice $G_1 \cdot G_2$ of two MMC graphs.

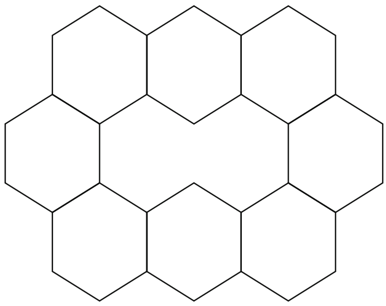


Figure 7. Graph $G_{1,0}$.

Lemma 5. Let $G_{m_i,k_i} \in \mathcal{G}_{m_i,k_i}$ for $i = 1, 2$. Then

$$G_{m_1,k_1} \cdot G_{m_2,k_2} \in \mathcal{G}_{m_1+m_2,k_1+k_2}.$$

Proof. Each splicing produces two new interior vertices, one of them black, the other one white. Hence the skewness of the splice is the sum of the skewnesses of its components. As the number of holes in the components is not affected by the splicing operation, and the only overlapping parts are the exposed hexagons, the claim follows. □

The graph $G_{1,0}$ shown in figure 7 is not a *sensu stricto* MMC graph, but its splice with an MMC graph from $\mathcal{G}_{m,k}$ will obviously result in an MMC graph from $\mathcal{G}_{m+1,k}$. We need $G_{1,0}$ as the starting point for a recursive definition of three infinite families of MMC graphs with low skewness.

Let $m \geqslant 3$ be a positive integer. By defining the graphs $G_{m,k}$ recursively as $G_{m,k} = G_{m-2,0} \cdot G_{2,k}$ for $k = 0, 1, 2$ we can demonstrate that there are MMC graphs with low skewness and arbitrary many holes.

Lemma 6. Let $m \geqslant 2$ be a positive integer. Then $\mathcal{G}_{m,k} \neq \emptyset$ for $k = 0, 1, 2$.

Now we can easily prove that k interpolates between 0 and $2m-2$.

Lemma 7. Let $m \geqslant 2$ be a positive integer. Then $\mathcal{G}_{m,k} \neq \emptyset$ for all $0 \leqslant k \leqslant 2m-2$.

Proof. The cases $k = 0, 1$, and 2 follow from lemma 6, and the case $k = 2m-2$ from lemma 4. Let now k be an even integer, $4 \leqslant k \leqslant 2m-4$. We set $k = 2i$ and construct the graph $G_{i+1,2i} \in \mathcal{G}_{i+1,2i}$ as in lemma 4. Then the splice $G_{i+1,2i} \cdot G_{m-i-1,0}$ is in $\mathcal{G}_{m,k}$, via lemma 5, and hence $\mathcal{G}_{m,k} \neq \emptyset$. For an odd k, $3 \leqslant k \leqslant 2m-3$, we set $k = 2i+1$. First, we construct $G_{i+1,2i} \in \mathcal{G}_{i+1,2i}$ and then we splice it with $G_{m-i-1,1}$. By lemma 5, the resulting graph is in $\mathcal{G}_{m,k}$, and hence $\mathcal{G}_{m,k} \neq \emptyset$. □

The proof of theorem 1, and hence both conjectures from [1] now follows by combining lemmas 3 and 7.

Acknowledgment

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