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Perfect Matchings in Hexagonal Systems

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Abstract. This paper deals with perfect matchings in hexagonal systems. Counterexamples are given to Sachs's conjecture in this field. A necessary and sufficient condition for a hexagonal system to have a perfect matching is obtained.

We follows the terminology and notation of Sachs [1]. A hexagonal unit cell is a plane region bounded by a regular hexagon of side length 1. A *hexagonal system* (HS) is a finite connected plane graph with no cut-vertices in which every interior region is a hexagonal unit cell.

Let H be a HS drawn in the plane. A straight line segment C with end points P_1, P_2 is called a *cut segment* of H, if it satisfies:

(1) C is orthogonal to one of the three edge directions of H.
(2) Each of P_1, P_2 is the center of an edge.
(3) Every point of C is either an interior or a boundary point of some unit cell of H.
(4) The graph obtained from H by deleting all edges intersected by C has exactly two components (see Fig. 1).

Let **C** denote the set of edges of H intersected by C; **C** is called an (elementary, orthogonal) *cut* of H.

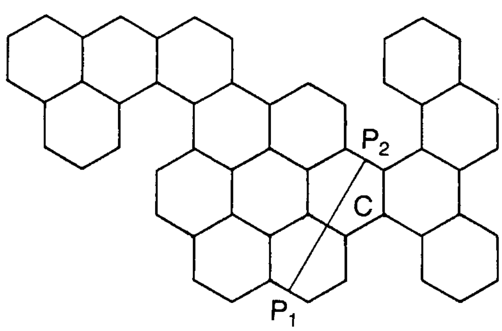

Fig. 1

Let C be a cut segment of H with associated cut **C**. Assume that H is drawn in such a way that C is horizontal. The component of H–**C** lying at the upper bank of C is denoted by $U(\mathbf{C})$.

We divide the vertices of H which are not incident with vertical edges into *peaks* and *valleys*: those of the form $\wedge$ are called peaks and those of the form $\vee$ are called valleys. Let $p(H)(v(H))$ denote the number of peaks (valleys) of H, and let $p(H/U(\mathbf{C}))(v(H/U(\mathbf{C})))$ be the number of peaks (valleys) of H which belong to $U(\mathbf{C})$.

A *perfect matching* (PM) of a graph G is a set of disjoint edges of G covering all vertices of G.

The problem of perfect matchings in a HS is of chemical relevance since a HS is the skeleton of a benzenoid hydrocarbon molecule if and only if it has a PM. Finding satisfactory necessary and sufficient conditions for the existence of PMs in a HS has been thought to be one of the most difficult open problems in the topological theory of HSs [2].

In [1] Sachs gave the following necessary condition for a HS H to have a PM:

If H has a PM, then for each of the six possible positions of H, (i) $p(H) = v(H)$ (ii) $0 \leq p(H/U(\mathbf{C})) - v(H/U(\mathbf{C})) \leq |\mathbf{C}|$, where **C** runs through all horizontal cuts.

Furthermore he formulated a conjecture:

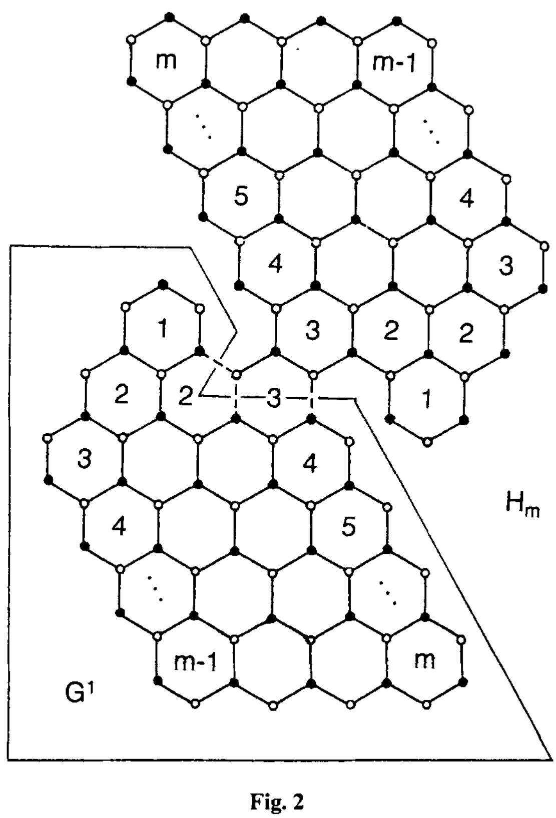

Fig. 2

Conjecture 1. If a HS H satisfies the above conditions (i) and (ii) for every horizontal cut and each of its six possible possitions, then H has a PM.

In fact this conjecture is invalid. We can construct infinitely many counter-examples to this conjecture.

Let H_m ($m \geq 4$) be given in Fig. 2. Then it is easy to see that H_m satisfies the above two conditions. But H_m has no PMs. At the end of this paper we shall see why this is so.

In what follows we assume that the vertices of a HS in question have been colored white and black. By $B(H)$ and $W(H)$ we denote the sets of black vertices and white vertices, respectively. Evidently $(B(H), W(H))$ is a bipartition of the vertex set of H.

An *edge-cut* (EC) of a HS H is a collection of edges of H such that the subgraph H − EC obtained from H by deleting all edges in EC has more components than H.

For a subset S of vertex set of graph G, we define the *neighbour set* of S in G to be the set of all vertices adjacent to vertices in S; this set is denoted by $N(S)$. For a nonempty subset of the vertex set of graph G, the subgraph of G whose vertex set is S and whose edge set is the set of those edges of G that have both ends in S is called the subgraph of G induced by S and is denoted by $\langle S \rangle$.

Theorem. *Let H be a HS such that $|B(H)| = |W(H)|$. Then H has a PM if and only if for each edge-cut $EC = \{e_1, \dots, e_t\}$ satisfying the following three conditions, we have $|B(G')| \geq |W(G')|$.*

(1) *H-EC has exactly two components G' and G''.*
(2) *The end vertex in G' of each e_i, $i = 1, \dots, t$, has the same colour, that is $V(EC) \cap V(G') \subset B(H)$, or $\subset W(H)$, where $V(EC)$ is the set of end vertices of edges in EC.*
(3) *Edges e_1 and e_t lie on the boundary of H, and e_i and e_{i+1} are edges of some hexagonal unit cell for every i, $1 \leq i \leq t - 1$.*

Proof. Suppose that H has a PM. For any edge-cut EC satisfying the above conditions (1)–(3), we may assume $V(\mathrm{EC}) \cap V(G') \subset B(H)$, and let $S = W(G')$. Since EC is an edge-cut of G, and $V(\mathrm{EC}) \cap V(G') \subset B(H)$, we have $N(S) = B(G')$. Since H has a PM, we have $|S| = |W(G')| \leq |B(G')| = |N(S)|$.

Conversely, if H has no PMs, by Hall's Theorem [3], there exists a subset S of $W(H)$ with $|S| > |N(S)|$. (If $|S| \leq |N(S)|$ for all $S \subset V(H)$, then H has a PM.) Since $|B(H)| = |W(H)|$, we have $S \neq W(H)$. It is clear that we can choose such a S so that the induced subgraph $\langle S \cup N(S) \rangle$ is connected. Furthermore we assume that S is maximal, i.e., S is not a proper subset of any subset S^* of $W(H)$ with $|S^*| > |N(S^*)|$. With the above conventions, it follows that $|S| = |N(S)| + 1$. (Otherwise, if $|S| > |N(S)| + 1$, we can take a vertex v which is not in S and is adjacent to a vertex in $N(S)$ and let $S' = S \cup \{v\}$. Since the degree of $v \leq 3$, we have $|N(S')| \leq |N(S)| + 2 < |S| + 1 = |S'|$. This contradicts the maximality of S.) Let $G' = \langle S \cup N(S) \rangle$ and $G'' = \langle V(H) - S \cup N(S) \rangle$. Then the edges with one end vertex in $V(G')$ and the other end vertex in $V(G'')$ form an edge-cut EC of H. It is easy to see that any edge in EC must be incident with a vertex of $N(S)$ in G'. Thus $V(\mathrm{EC}) \cap V(G') \subset B(H)$.

Now we show that G'' is connected. Since $|B(H)| = |W(H)|$ and $|B(G')| = |W(G')| - 1$, we have $|W(G'')| = |B(G'')| - 1$. Let $G''_1, G''_2, \dots, G''_p$ be the components of G''. Then we have

$$|B(G'')| - |W(G'')| = \sum_{i=1}^{p} (|B(G_i'')| - |W(G_i'')|) = 1.$$

On the other hand we have $|B(G_i'')| - |W(G_i'')| \geq 1$ by the maximality of $S = W(G')$. Hence $p = 1$ and thus G'' is connected.

Suppose $\langle S \cup N(S) \rangle$ has no vertices in the boundary of H. Then $\langle S \cup N(S) \rangle$ is surrounded by hexagons of H. By Lemma 2.3 in [2], there is a white vertex of degree 2 in the boundary of $\langle S \cup N(S) \rangle$ and the edge of H incident with the vertex belongs to EC, which is contrary to $V(\mathrm{EC}) \cap V(G') \subset B(H)$. Hence some of the vertices in $\langle S \cup N(S) \rangle$ must lie on the boundary of H.

Since $\langle S \cup N(S) \rangle$ contains edges in the boundary of H, and $H - \mathrm{EC}$ has exactly two components G' and G'', the edge-cut EC must contain at least two boundary edges, say e_1 and e_t, and the edges e_i and e_{i+1} are the edges of some hexagonal unit cell for every i, $1 \leq i \leq t-1$.

Thus if H has no PMs, there exists an edge-cut EC satisfying the above conditions (1)–(3), and $|B(G')| = |N(S)| = |S| - 1 = |W(G')| - 1 < |W(G')|$, i.e., $|B(G')| < |W(G')|$.

Consequently, the theorem is proved.

Now we prove that H_m has no PMs by using the above theorem. Let EC be the set of edges indicated by dash lines (see Fig. 2). Then EC satisfies the three conditions in Theorem, but $|B(G')| < |W(G')|$. Hence H_m has no PMs.

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