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A Maximal Alternating Set of a Hexagonal System

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Abstract

We show that for a maximal alternating set P of a hexagonal system H, H-P is empty or has a unique perfect matching.

1. Introduction

Let C be a cycle on the hexagonal lattice. Then the vertices and the edges of the hexagonal lattice which lie on C and in the interior of C form a hexagonal system [1]. The vertices of a hexagonal system H are divided into external and

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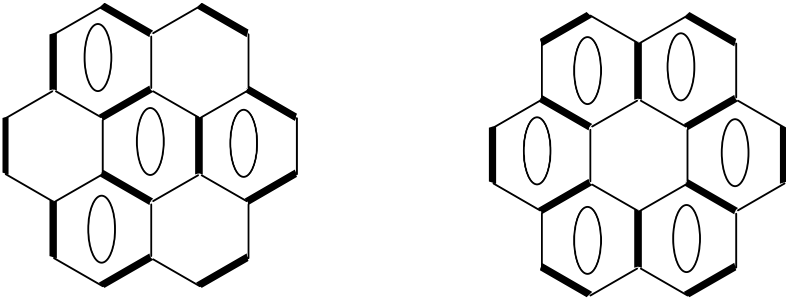
internal. A vertex of H lying on the boundary of the exterior face of H is called an external vertex, otherwise, it is called an internal vertex. A hexagon of H such that none of its vertices is external is called an internal hexagon, otherwise, it is an external hexagon. If a hexagonal system has no internal vertices, it said to be catacondensed, otherwise, it is pericondensed. A pericondensed hexagonal system is fat if it has an internal hexagon, otherwise, it is thin. A hexagonal system is to be placed on the plane so that a pair of edges of each hexagon lies in parallel with the vertical axis. A perfect matching of a hexagon is called a sextet [2]. It is proper if the right vertical edge of the hexagon is in the perfect matching; otherwise, it is improper.

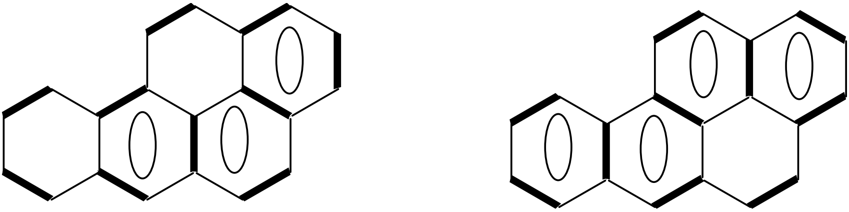
Let P be a non-empty set of hexagons of a hexagonal system H. We call P a set of mutually alternating hexagons of H (or simply an alternating set or a framed set) if there exists a perfect matching of H that contains a sextet of each hexagon in P [3]. An alternating set is maximal if it is not contained in a larger alternating set. An alternating set is maximum if its cardinality is the largest among all alternating sets. As Fig.1 shows, a maximal alternating set is not necessarily maximum. The cardinality of a maximum alternating set is of significance in the chemistry of benzenoid hydrocarbons [4]. It is called the Fries number [5].

Let H be a hexagonal system and P a non-empty set of hexagons. H-P denotes the subgraph of H obtained by deleting from H the vertices of the hexagons in P (together with their incident edges).



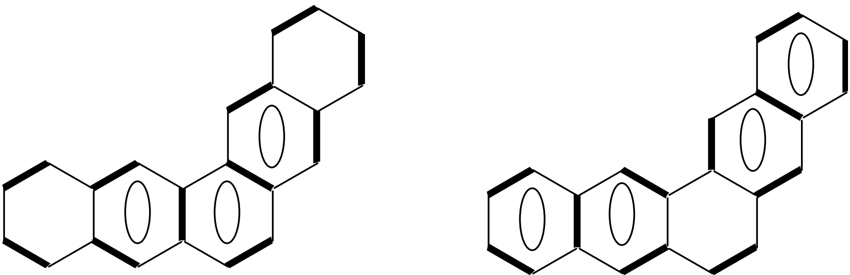
A maximal alternating set | A maximum alternating set

FIGURE 1-a: Coronene, a fat pericondensed hexagonal system.



A maximal alternating set | A maximum alternating set

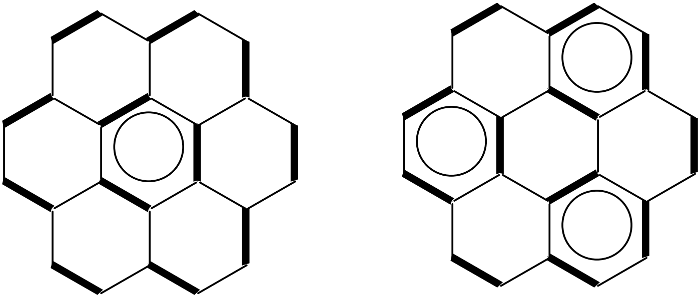
FIGURE 1-b: benzo[a]pyrene, a thin pericondensed hexagonal system.



A maximal alternating set | A maximum alternating set

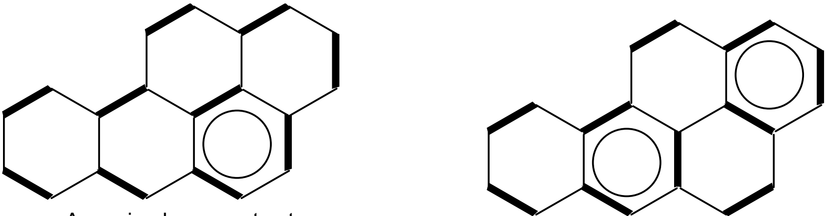
FIGURE 1-c: A catacondensed hexagonal system.

Let P be a non-empty set of hexagons of a hexagonal system H. We call P a resonant set of H if the hexagons in P are pair-wise disjoint and there exists a perfect matching of H that contains a sextet of each hexagon in P [3] or equivalently [6] if the hexagons in P are pair-wise disjoint and H-P has a perfect matching or is empty. A resonant set is maximal if it is not contained in a larger resonant set. A resonant set is maximum if its cardinality is the largest among all resonant sets. As Fig. 2 shows, a maximal resonant set is not necessarily maximum. The cardinality of a maximum resonant set is of significance in the chemistry of benzenoid hydrocarbons [7]. It is called the Clar number [8].



A maximal resonant set
A maximum resonant set

FIGURE 2-a: Coronene, a fat pericondensed hexagonal system.



A maximal resonant set
A maximum resonant set

FIGURE 2-b: benzo[a]pyrene, a thin pericondensed hexagonal system.

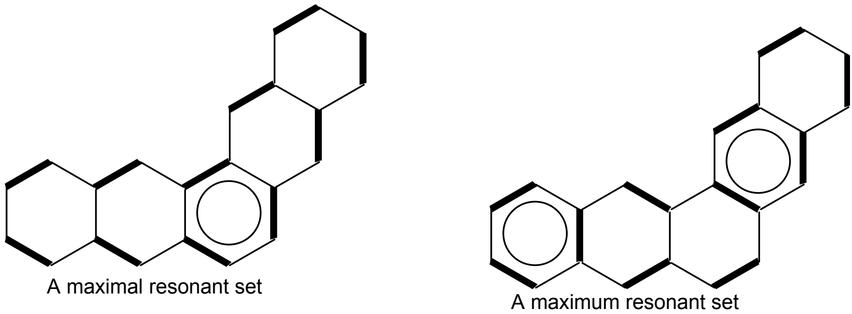


FIGURE 2-c: A catacondensed hexagonal system.

If H is a catacondensed hexagonal system and P is a maximal resonant set then H-P is empty or has a unique perfect matching [6]. Counterexamples [6] show that the statement cannot be extended to pericondensed hexagonal systems. If H is a pericondensed hexagonal system and P is a maximum resonant set then H-P is empty or has a unique perfect matching [9]. This statement was conjectured by Gutman [10].

If H is a catacondensed hexagonal system and P is a maximal alternating set then H-P is empty or has a unique perfect matching [11]. The aim of this paper is to prove this result for any hexagonal system (Theorem 5). Those interested in only catacondensed hexagonal systems are referred to [11] since the proof given there is simpler than that given here. A basic related result is that if H is a hexagonal system and P is an alternating set then H-P is empty or has a perfect matching. This basic result was mentioned in [11] without proof and here we include it as Lemma 1 and a proof is given.

If G is a subgraph of H, we use H-G to denote the subgraph of H obtained by deleting from H all the vertices of G (together with the incident edges).

2. Results

Lemma 1. Let P be an alternating set of a hexagonal system H. Then H-P is empty or has a perfect matching.

Proof. We can assume that H-P is non-empty. Let M be a perfect matching of H that contains a sextet of each hexagon in P. let $M^*=\{e \in M$: e is not contained in a hexagon in P$\}$. It is clear that M* is a perfect matching of H-P. **Q.E.D.**

Lemma 2. Let P be an alternating set of a hexagonal system H such that H-P is not empty. Then a perfect matching of H-P can be extended to a perfect matching of H that contains a sextet of each hexagon in P.

Proof. Let M_1 be a perfect matching of H-P. Let M be a perfect matching of H that contains a sextet of each hexagon in P. Let $M_2=\{e \in M$: e is contained in a hexagon in P$\}$. It can be seen that $M_1 \cup M_2$ is a perfect matching of H that contains a sextet of each hexagon in P. **Q.E.D.**

Lemma 3. Let H be a hexagonal system, P be an alternating set of H consisting of internal hexagons and ∂H be the cycle of the boundary of the exterior face of H. If (H-P)-∂H is empty or has a perfect matching then P is not a maximal alternating set.

Proof. The proof of this Lemma is that of a related result by Zheng and Chen [9] with modifications.

If (H-P)-∂H is empty, let M be the empty set, otherwise, let M be a perfect matching of (H-P)-∂H. The edges of ∂H can be decomposed into two perfect matchings N_1 and N_2 of ∂H since ∂H is an even cycle. It is clear that $M \cup N_1$ and $M \cup N_2$ are two perfect matchings of H-P.

We assume that P is a maximal alternating set and then derive a contradiction.

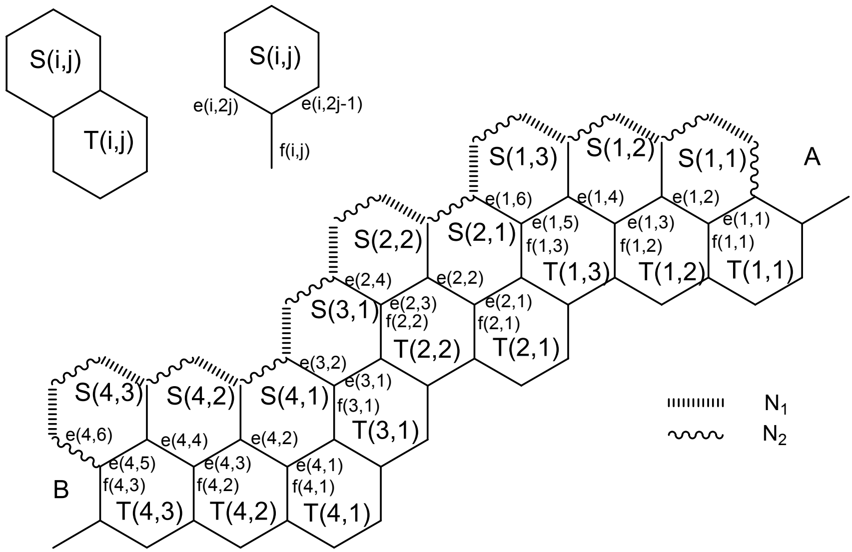


FIGURE 3: Hexagons S(i,j) and T(i,j) and edges f(i,j) and e(i,k) with m=4, n(1)=3, n(2)=2, n(3)=1 and n(4)=3

Let {S(i,j): 1 ≤ i ≤ m, 1 ≤ j ≤ n(i)} be the series of hexagons of the hexagonal system H which lies on the boundary of the exterior face of H and satisfies that neither hexagon A nor hexagon B is a hexagon of H as shown in Fig. 3. The series of hexagons of the hexagonal lattice $\{T(i,j): 1 \leq i \leq m, 1 \leq j \leq n(i)\}$ are as shown in Fig. 3. T(i,j) may be a hexagon of the hexagonal system H. The vertical edges f(i,j), $1 \leq i \leq m$, $1 \leq j \leq n(i)$ and the diagonal edges e(i,k), $1 \leq i \leq m$, $1 \leq k \leq 2n(i)$ are as shown in Fig. 3.

We first show that the following three statements hold by induction on i.

(a) $m \geq 2$ and $n(i) = 1$ or $n(i) = 2$ for all i, $1 \leq i \leq m$.

(b) if n(i) =1 then $f(i,1) \in M$.

(c) if n(i) =2 then $T(i,2) \in P$.

Initial Step: We prove that the above statements hold for i=1.

(a) Assume that $n(1) \geq 3$.

Case: $T(1,1) \notin H$ and $T(1,2) \notin H$. By Lemma 2, $P \cup \{S(1,1)\}$ is an alternating set of H, a contradiction.

Case: $T(1,1) \notin H$ and $T(1,2) \in H$. $T(1,2) \notin P$ since $T(1,1) \notin H$. Hence $e(1,3) \in M$. Consequently, $e(1, 2n(1)-1) \in M$. By Lemma 2, $P \cup \{S(1,n(1))\}$ is an alternating set, a contradiction.

Case: $T(1,1) \in H$ and $T(1,2) \notin H$. $e(1,2) \in N_2$, say. By Lemma 2, $P \cup \{S(1,1)\}$ is an alternating set, a contradiction.

Case: $T(1,1) \in H$ and $T(1,2) \in H$. *Subcase:* $e(1,2) \in M$. By Lemma 2, $P \cup \{S(1,1)\}$ is an alternating set, a contradiction. *Subcase:* $e(1,3) \in M$. Then $e(1, 2n(1)-1) \in M$. By Lemma 2, $P \cup \{S(1,n(1))\}$ is an alternating set, a contradiction. *Subcase:* $e(1,2) \notin M$ and $e(1,3) \notin M$. $T(1,2) \in P$. Hence $T(1,3) \in H$. If $T(1,3) \in P$, then in the extended perfect matching mentioned in Lemma 2, T(1,2) is an improper sextet, thus, e(1,2) is matched and $P \cup \{S(1,1)\}$ is an alternating set, a contradiction. If $T(1,3) \notin P$, then e(1,2n(1)-1) ∈ M and by Lemma 2, P ∪ {S(1, n(1))} is an alternating set, a contradiction.

Consequently, we have n(1) ≤ 2.

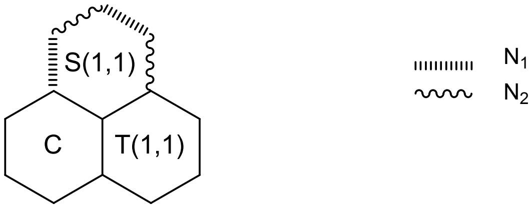


FIGURE 4: Proof of Lemma 3.

(b) n(1) = 1. See Fig. 4. Assume that T(1,1) ∉ H. Then, by Lemma 2, P ∪ {S(1,1)} is an alternating set, a contradiction. Hence, T(1,1) ∈ H. T(1,1) ∉ P. Assume that C ∉ H. Then e(1,2) ∈ N_2, say, and by Lemma 2, P ∪ {S(1,1)} is an alternating set, a contradiction. Hence C ∈ H and can be denoted by S(2, 1) (from which m ≥ 2). Thus, f(1,1) ∈ M.

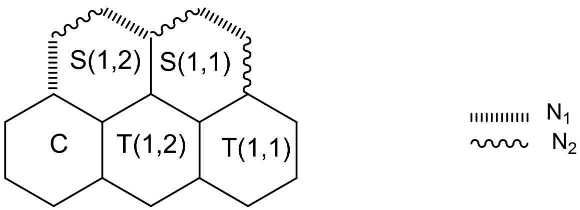


FIGURE 5: Proof of Lemma 3.

(c) $n(1) = 2$. See Fig. 5. Assume that $T(1,2) \notin H$. Then $e(1,2) \in N_2$, say. By Lemma 2, $P \cup \{S(1,1)\}$ is an alternating set, a contradiction. Hence $T(1,2) \in H$.

Assume that $T(1,2) \notin P$. *Case:* $e(1,2) \in M$. By Lemma 2, $P \cup \{S(1,1)\}$ is an alternating set, a contradiction. *Case:* $e(1,3) \in M$. By Lemma 2, $P \cup \{S(1,2)\}$ is an alternating set, a contradiction. Hence, $T(1,2) \in P$. It follows that $C \in H$ and can be denoted by $S(2,1)$. Thus, $m \geq 2$.

Consequently, $m \geq 2$ and the statements hold for $i=1$.

Inductive Step: We assume that the statements hold for $i=r-1$ and prove that they hold for $i=r$, where $2 \leq r \leq m$.

Case: $n(r-1) = 1$. We have $f(r-1, 1) \in M$.

(a) Assume that $n(r) \geq 3$. See Fig. 6.

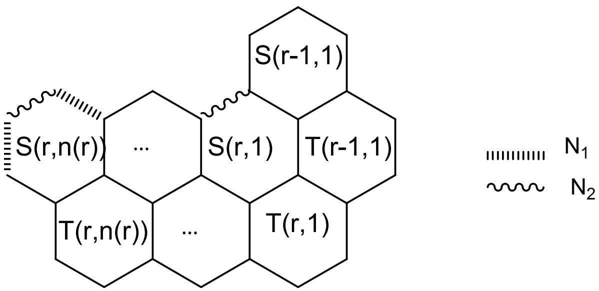


FIGURE 6: Proof of Lemma 3.

Case: $T(r, n(r)) \in H$ and $T(r, n(r)) \in P$. $T(r, n(r)-1) \in H$. *Subcase:* $T(r, n(r)-1) \in P$. Then an extended perfect matching of Lemma 2 contains a proper sextet of $T(r, n(r))$ and $P \cup \{S(r, n(r))\}$ is an alternating set, a contradiction. *Subcase:* $T(r, n(r)-1) \notin P$. Then $e(r, 2) \in M$ and by Lemma 2, $P \cup \{S(r, 1)\}$ is an alternating set, a contradiction.

Case: T(r, n(r)) $\in$ H and T(r, n(r)) $\notin$P. *Subcase:* e(r, 2n(r)-1) $\in$ M. Then by Lemma 2, P $\cup$ {S(r, n(r))} is an alternating set, a contradiction. *Subcase:* e(r, 2n(r)-2) $\in$ M. Then e(r, 2) $\in$ M and by Lemma 2, P $\cup$ {S(r, 1)} is an alternating set, a contradiction.

Case: T(r, n(r)) $\notin$ H. e(r, 2n(r)-1) $\in$ N_1, say. By Lemma 2, P $\cup$ {S(r, n(r))} is an alternating set, a contradiction.

Hence, n(r) ≤ 2.

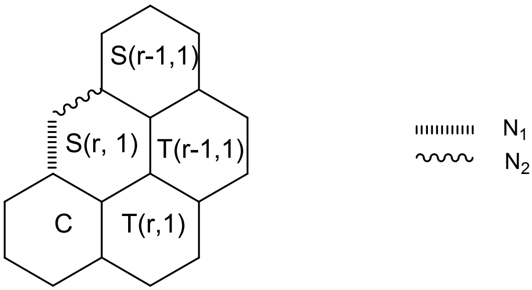


FIGURE 7: n(r-1)= 1, n(r)= 1.

(b) n(r) = 1. See Fig. 7. T(r, 1) $\in$ H and T(r, 1) $\notin$ P since f(r-1, 1) $\in$ M. Assume that C $\notin$ H. Then by Lemma 2, P $\cup$ {S(r, 1)} is an alternating set, a contradiction. Hence, C $\in$ H and can be denoted by S(r+1, 1). Thus, f(r, 1) $\in$ M.

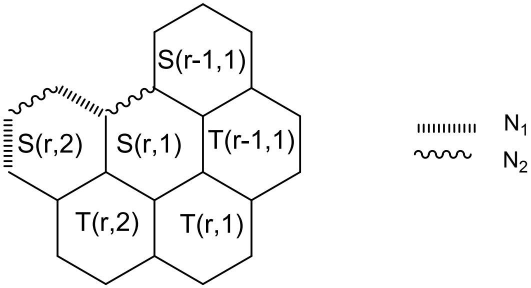


FIGURE 8: n(r-1)=1, n(r)=2.

(c) n(r)= 2. See Fig. 8. Assume that T(r, 2) $\notin$ H. Then e(r, 2) $\in$ N_2, say, and by Lemma 2, P $\cup$ {S(r, 1)} is an alternating set, a contradiction. Hence, T(r, 2) $\in$ H.

Assume that T(r, 2) $\notin$ P. *Case:* e(r, 2) $\in$ M. By Lemma 2, P $\cup$ {S(r, 1)} is an alternating set, a contradiction. *Case:* e(r, 3) $\in$ M. By Lemma 2, P $\cup$ {S(r, 2)} is an alternating set, a contradiction. Hence, T(r, 2) $\in$ P.

Case: n(r-1) = 2. We have T(r-1, 2) $\in$ P.

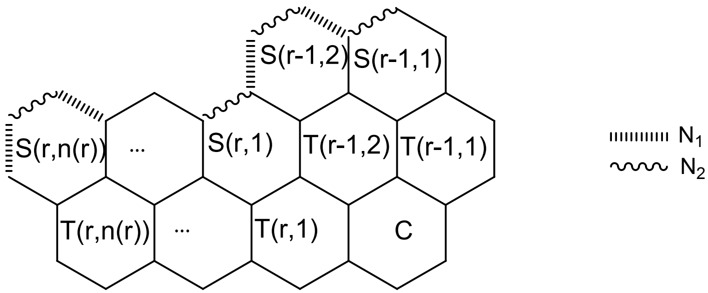


FIGURE 9: Proof of Lemma 3.

(a) Assume that $n(r) \geq 3$. See Fig. 9.

Case: $T(r, n(r)) \in H$ and $T(r, n(r)) \in P$. $T(r, n(r)-1) \in H$. *Subcase:* $T(r, n(r)-1) \in P$. Then an extended perfect matching of Lemma 2 contains a proper sextet of $T(r, n(r))$ and $P \cup \{S(r, n(r))\}$ is an alternating set, a contradiction. *Subcase:* $T(r, n(r)-1) \notin P$. Then $e(r, 2) \in M$. If $T(r-1, 1) \in P$ then an extended perfect matching of Lemma 2 contains a proper sextet of $T(r-1, 2)$ and $P \cup \{S(r-1, 2)\}$ is an alternating set, a contradiction. If $T(r-1, 1) \notin P$, note that $T(r, 1) \notin P$ since $e(r,2) \in M$, thus, none of the hexagons that are adjacent to $T(r-1, 2)$ belongs to P except possibly hexagon C. Hence, an extended perfect matching of Lemma 2 contains an improper sextet of $T(r-1, 2)$ and $P \cup \{S(r, 1)\}$ is an alternating set, a contradiction.

Case: $T(r, n(r)) \in H$ and $T(r, n(r)) \notin P$. *Subcase:* $e(r, 2n(r)-1) \in M$. By Lemma 2, $P \cup \{S(r, n(r))\}$ is an alternating set, a contradiction. *Subcase:* $e(r, 2n(r)-2) \in M$. Then $e(r, 2) \in M$. If $T(r-1, 1) \in P$, then an extended perfect matching of Lemma 2 contains a proper sextet of $T(r-1, 2)$ and $P \cup \{S(r-1, 2)\}$ is an alternating set, a contradiction. If $T(r-1, 1) \notin P$, note that $T(r, 1) \notin P$ since $e(r,2) \in M$, thus, none of the hexagons that are adjacent to $T(r-1, 2)$ belongs to P except possibly hexagon C. Hence, an extended perfect matching of Lemma 2 contains an improper sextet of $T(r-1, 2)$ and $P \cup \{S(r, 1)\}$ is an alternating set, a contradiction.

Case: $T(r, n(r)) \notin H$. $e(r, 2n(r)-1) \in N_1$, say. By Lemma 2, $P \cup \{S(r, n(r))\}$ is an alternating set, a contradiction.

Hence, $n(r) \leq 2$.

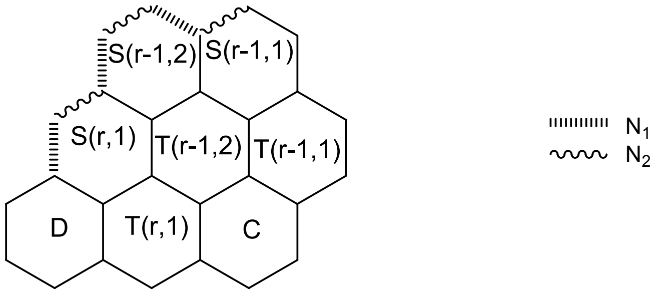


FIGURE 10: n(r-1)=2, n(r)=1.

(b) n(r) = 1. See Fig. 10. Assume that either T(r, 1) or T(r-1, 1) belongs to P. Then, an extended perfect matching of Lemma 2 contains a proper sextet of T(r-1, 2) and P $\cup$ {S(r-1, 2)} is an alternating set, a contradiction. Hence, neither T(r, 1) nor T(r-1, 1) belongs to P.

Assume that D $\notin$ H. Then e(r, 2) $\in$ N_2, say. Note that none of the hexagons that are adjacent to T(r-1, 2) belongs to P except possibly hexagon C. Hence, an extended perfect matching of Lemma 2 contains an improper sextet of T(r-1, 2) and P $\cup$ {S(r, 1)} is an alternating set, a contradiction. Hence, D $\in$ H and can be denoted by S(r+1, 1). Note that T(r, 1) $\in$ H since T(r-1, 2) $\in$ P. Recall that T(r, 1) $\notin$ P. Thus, f(r, 1) $\in$ M.

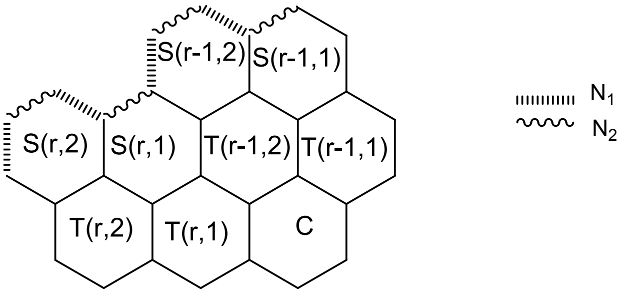


FIGURE 11: n(r-1)=2, n(r) =2.

(c) n(r) = 2. See Fig. 11. Assume that T(r, 2) $\notin$ H. Then e(r, 3) $\in$ N_1, say, and by Lemma 2, P $\cup$ {S(r, 2)} is an alternating set, a contradiction. Hence, T(r, 2) $\in$ H.

Assume that T(r, 2) $\notin$ P. *Case:* e(r, 2) $\in$ M. T(r, 1) $\notin$ P. *Subcase:* T(r-1, 1) $\in$ P. Then an extended perfect matching of Lemma 2 contains a proper sextet of T(r-1, 2) and P $\cup$ {S(r-1, 2)} is an alternating set, a contradiction. *Subcase:* T(r-1, 1) $\notin$ P. Then none of the hexagons that are adjacent to T(r-1, 2) belongs to P except possibly hexagon C. Hence, an extended perfect matching of Lemma 2 contains an improper sextet of T(r-1, 2) and P $\cup$ {S(r, 1)} is an alternating set, a contradiction. *Case:* e(r, 3) $\in$ M. By Lemma 2, P $\cup$ {S(r, 2)} is an alternating set, a contradiction. Hence, T(r, 2) $\in$ P.

By induction, the three statements hold. The statements for i=m imply that hexagon B is a hexagon of H, a contradiction. **Q.E.D.**

Lemma 4 [10]**.** Every perfect matching of a hexagonal system contains a sextet of a hexagon.

Theorem 5. Let H be a hexagonal system and P a maximal alternating set of H. Then H-P is empty or has a unique perfect matching.

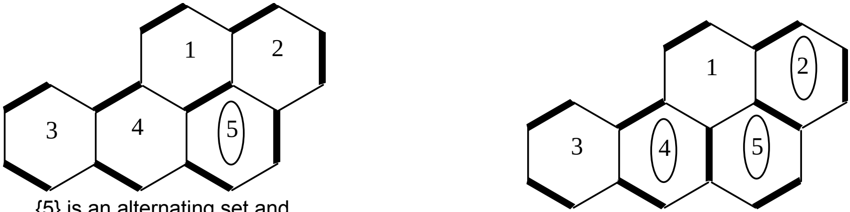
Proof. The proof of this theorem is that of a related result by Zheng and Chen [9] with modifications**.**

We can assume that H-P is not empty. That H-P has a perfect matching follows from Lemma 1. Assume that H-P has more than one perfect matching. Let M and M' be two perfect matchings of H-P. Then the symmetric difference $M \oplus M' = (M \cup M') - (M \cap M')$ contains an (M, M')-alternating cycle C, say. The vertices and the edges of the hexagonal lattice which lie on C and in the interior of C form a hexagonal system H*, say. Since C is a cycle of H, H* is a subgraph of H. Let N be the set of hexagons of H* and $P^* = P \cap N$. M is a perfect matching of H-P and so, by Lemma 2, it can be extended to a perfect matching M_{ext} of H that contains a sextet of each hexagon in P.

$M_{ext} \cap E(H^*)$ is a perfect matching of H* that contains a sextet of each hexagon in P* and $\partial H^*=C$ is alternating in it. Thus, if $P^* \neq \emptyset$, it is an alternating set of H* consisting of internal hexagons (since C is in H-P) and $(H^*-P^*)-\partial H^*$ is empty or has a perfect matching. Let P^*_{ext} be an alternating set of H* that contains P* as a proper subset. The existence of P^*_{ext} follows from Lemma 3 if $P^* \neq \emptyset$ and from Lemma 4 if $P^* = \emptyset$. Let M* be a perfect matching of H* that contains a sextet of each hexagon in P^*_{ext}.

$M^* \cup (M_{ext} - E(H^*))$ is a perfect matching of H and it contains a sextet of each hexagon in $P^*_{ext} \cup (P - P^*)$ since C is a cycle of H-P. Thus, $P^*_{ext} \cup (P - P^*)$ is an alternating set of H that contains P as a proper subset, a contradiction. **Q.E.D.**

Remark. If H is a hexagonal system, P an alternating set of H and H-P is empty or has a unique perfect matching, then P is not necessarily a maximal alternating set. For a counterexample, see Fig. 12.



{5} is an alternating set and
H-{5} has a unique perfect matching

{5} is not a maximal alternating set

FIGURE 12: A counterexample.

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