

Continuous forcing spectra of perfect matchings of convex hexagonal systems*

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Abstract

A convex hexagonal system is a hexagonal system whose inner dual graph has a convex polygonal boundary. A forcing set S for a perfect matching M of a graph G is a subset of M that is contained in no other perfect matchings of G . The smallest cardinality of a forcing set of M is called the forcing number of M , denoted by $f(G, M)$. The forcing spectrum of G is defined as: $\text{Spec}(G) = \{f(G, M) | M \text{ is a perfect matching of } G\}$. In this paper, we show that for any convex hexagonal system $O(m, k, n)$ with a perfect matching, its forcing spectrum is continuous (or an integer interval).

Keywords: Convex hexagonal system, perfect matching, forcing number, forcing spectrum.

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1 Introduction

A hexagonal system (or benzenoid system) H is a plane 2-connected bipartite graph whose interior faces are regular hexagons with length 1. A perfect matching (or Kekulé structure in chemical literature) M of a graph G is a set of disjoint edges covering all vertices of G . A forcing set of a perfect matching M of a graph G is a subset S of M that is contained in no other perfect matchings of G . The smallest cardinality of a forcing set of M is called the forcing number of M , denoted by $f(G, M)$. The minimum (resp. maximum) forcing number of G is the minimum (resp. maximum) value of forcing numbers of all perfect matchings of G , denoted by $f(G)$ (resp. $F(G)$).

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The forcing number of a perfect matching of a graph was introduced by Harary et al. [7], and originally appeared in earlier papers of Randić and Klein [8, 11] under the name “innate degree of freedom” of Kekulé structures, which plays an important role in the resonance theory in chemistry. Xu et al. [14] proved that the maximum forcing number of a hexagonal system is equal to its Clar number, which can measure the stability of benzenoid hydrocarbons within Clar’s aromatic sextet theory [5]. For polyomino graphs and (4,6)-fullerene graphs, the same results still hold [13, 23] in an extensive sense.

A spanning subgraph C of a hexagonal system H is called a *Clar cover* if each component of C is either a hexagon or an edge. The set of hexagons of a Clar cover C of H is a *resonant set* or *sextet pattern* of H . Let $h(C)$ denote the number of hexagons of C . A Clar cover of H with the maximum number of hexagons is called a *Clar structure*, and the *Clar number* $Cl(H)$ of H is the number of hexagons in a Clar structure.

Afshani et al. [2] defined the *forcing spectrum* of a graph G as:

$$\text{Spec}(G) = \{f(G, M) \mid M \text{ is a perfect matching of } G\}$$

and showed that any finite set of positive integers can be the forcing spectrum of a planar bipartite graph. So it is an interesting problem to determine whether a graph G has the *continuous* forcing spectrum, i.e. $\text{Spec}(G)$ forms an integer interval from the minimum to maximum forcing numbers of G . Lam and Pachter [9] determined the forcing spectra of polyomino graphs of stop signs that are continuous. For any simply-connected polyomino graphs Zhang and Jiang [19] showed their forcing spectra are always continuous by using Z-transformation graph. Che and Chen [4] conjectured that the forcing spectrum of any fullerene graph is continuous. A hexagonal system is called *forced* if it has a forcing edge (an edge in exactly one perfect matching). Zhang and Li [17] determined the forced hexagonal systems. Zhang and Deng [18] further got the forcing spectra of forced hexagonal systems, which are either continuous or with only gap 2. For a recent survey on matching forcing and related topics, see [20].

The *inner dual graph* $T(H)$ of a hexagonal system H is a plane graph such that the vertices are the centers of all the hexagons of H , and two vertices are joined by a (straight) edge providing the corresponding hexagons have a common edge in H . The boundary of $T(H)$ means the boundary of the exterior face of $T(H)$. A hexagonal system H is *convex* if the boundary of $T(H)$ bounds a convex polygon or a straight line segment. Cyvin and Gutman [6] showed that a convex hexagonal system has a perfect matching if and only if the periphery of $T(H)$ is either a path, a parallelogram or a big hexagon with each angle equal to 120° and each pair of opposite sides having the same length. Therefore any convex hexagonal system with a perfect matching can be uniquely determined by an integer triplet (m, k, n) and denoted by $O(m, k, n)$ with conventions $m \leq k \leq n$; For example, see Figure 1.

For a convex hexagonal system $O(m, k, n)$, Cyvin and Gutman [6] and Bodroža et al. [3] gave and proved a formula for the number of Kekulé structures respectively. Zhang [17] got an expression of its Clar number, i.e. maximum forcing number. Zhang and Zhang [21] proved that its minimum forcing number is equal to m by using monotonic path systems. Further they [22] proved that a regular convex hexagonal system $O(m, m, m)$ has the continuous forcing spectrum.

In this paper we use a simpler method to show that the forcing spectrum of a general convex hexagonal system $O(m, k, n)$ is also continuous (see Theorem 3.6). To this end we give some preliminaries in Section 2 and a proof to our main result in Section 3.

2 Preliminaries

Suppose that hexagonal systems considered are drawn in the plane such that some edges are vertical. Let H be a hexagonal system with a specific hexagon s_0 at the center, O . We establish a 3-coordinate system $O - ABC$ on H such that O is the origin and the three axes are perpendicular to three disjoint edges of s_0 respectively (see Figures 1 and 2). The coordinate system $O - ABC$ divides the plane into three areas AOB , BOC and COA . For a point W in the plane, we define its coordinates with respect to $O - ABC$. If W lies in the area AOB (for the other cases we can do similarly), draw two straight lines through W such that one is parallel to axis OB and intersects axis OA at the point W_A , and the other is parallel to axis OA and intersects axis OB at the point W_B . Suppose that the distance between two centers of any two adjacent hexagons of H is 1. The lengths of OW_A and OW_B are defined as the coordinates of W on axes OA and OB respectively, and the coordinate of W on axis OC is defined as zero (see Figure 2). If the lengths of OW_A and OW_B are denoted by x and y respectively, then the coordinate of W with respect to $O - ABC$ is written as $(x, y, 0)$.

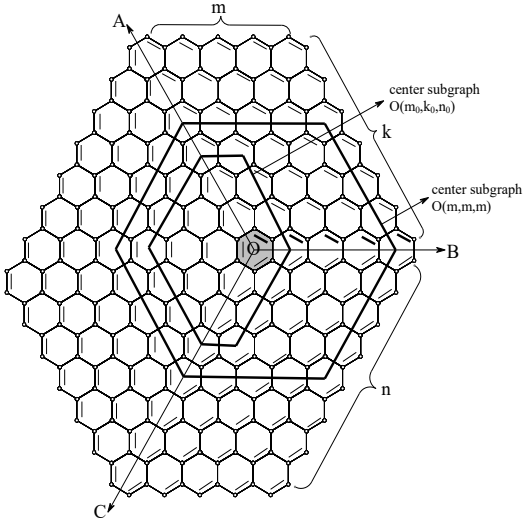


Figure 1. $O(5, 7, 8)$ with 3-divisible M and center subgraphs.

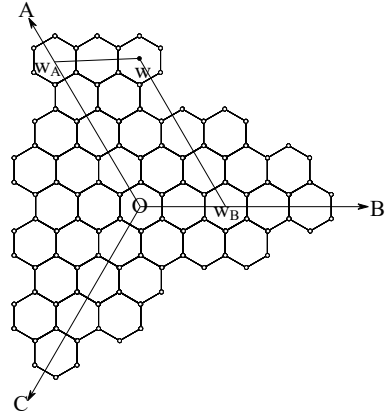


Figure 2. The coordinate $(4, 2, 0)$ of a point W w.r.t. $O - ABC$.

We mark a hexagon in H with $s_{i,j,k}$, where (i, j, k) is the coordinate of the center of the hexagon. We make a convention: we use double bonds, bold double bonds and grey hexagons to represent a perfect matching, a forcing set and the hexagons of a Clar cover, respectively.

A perfect matching M of a hexagonal system H is called 3-divisible if no edge of M intersect an axis and the edges of M lying in the same area are mutually parallel to each other (see Figure 1).

The Z -transformation graph or resonance graph $Z(H)$ of a hexagonal system H is the graph whose vertices represent the perfect matchings of H and two perfect matchings M_1 and M_2 of H are joined by an edge if and only if they differ in exactly one hexagon of H .

Lemma 2.1 ([16], Lemma 1). *Let H be a hexagonal system. Then $Z(H)$ has a 1-degree vertex if and only if there exists a 3-coordinate system $O - ABC$ w.r.t. a hexagon s_0 such that a perfect matching M of H is 3-divisible w.r.t. $O - ABC$.*

Zhang and Li [16] proved that $Z(O(m, k, n))$ has exactly two vertices of degree one. For convenience, from now on we always place an $O(m, k, n)$ on the plane and establish a 3-coordinate system $O - ABC$ w.r.t. s_0 satisfying the condition of Lemma 2.1 and axes OB , OA and OC toward right, upward and downward (see Figure 1).

Let M be a 3-divisible perfect matching of $O(m, k, n)$ w.r.t. $O - ABC$. A subgraph $O(m_0, k_0, n_0)$ of $O(m, k, n)$ is called a *center subgraph* ($1 \leq m_0 \leq m, m_0 \leq k_0 \leq k, k_0 \leq n_0 \leq n$) if $M \cap E(O(m_0, k_0, n_0))$ is also a 3-divisible perfect matching of $O(m_0, k_0, n_0)$ w.r.t. $O - ABC$ (see Figure 1).

Let G be a graph with a perfect matching. A subgraph G' of a graph G is called a *nice subgraph* of G if $G - V(G')$ has a perfect matching.

Proposition 2.2. *Any center subgraph $O(m_0, k_0, n_0)$ of $O(m, k, n)$ is a nice subgraph of $O(m, k, n)$.*

For a bipartite graph G with a perfect matching M , an edge subset $S \subset M$ forces an edge $uv \in M \setminus S$ if all neighbors of v except u are in $V(S)$, where $V(S)$ denotes the set of end-vertices of edges in S . If there exists a sequence of edges $\{e_i\}_{i=1}^k$ and a sequence of edge subsets $\{S_i\}_{i=0}^k$ such that $S_0 = S$, $S_i = S_{i-1} \cup \{e_i\}$ and S_{i-1} forces e_i for $1 \leq i \leq k$, then we say S forces S_k . We define $G \ominus S$ as $G - V(S_k)$ whenever S forces S_k and $G - V(S_k)$ has no 1-degree vertex.

Lemma 2.3 ([1, 12]). *Let M be a perfect matching of a bipartite graph G . Then S is a forcing set of M if and only if S forces M .*

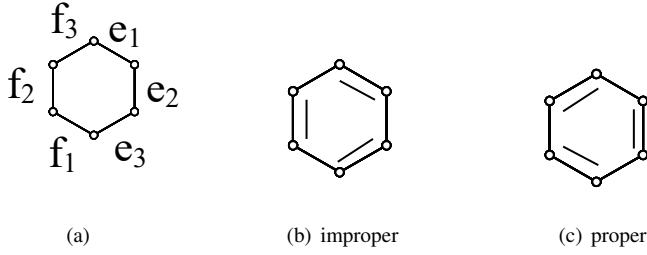
Proposition 2.4. *Let M be a perfect matching of a bipartite graph G . For any $S \subseteq M$, if S' is a forcing set of $E(G \ominus S) \cap M$ in the subgraph $G \ominus S$, then $S \cup S'$ is a forcing set of M .*

Proof. Since S' is a forcing set of $(G \ominus S) \cap M$, that is, $S \cup S'$ forces M . By Lemma 2.3, we have that $S \cup S'$ is a forcing set of M . $\square$

Let A and B be finite sets. Then we define the *symmetric difference* $A \triangle B = (A - B) \cup (B - A) = A \cup B - A \cap B$. Let M be a perfect matching of a graph G . A cycle of G is M -alternating, if its edges appear alternately in M or not. If C is an M -alternating cycle of G , then $M \triangle C := M \triangle E(C)$ is also a perfect matching of G . If $\mathcal{C} = \{C_1, C_2, \dots, C_m\}$ is a set of disjoint M -alternating cycles of G , then we define $M \triangle \mathcal{C} = M \triangle C_1 \triangle C_2 \triangle \dots \triangle C_m$ for convenience, which is also a perfect matching of G .

Lemma 2.5 ([10]). *Let M be a perfect matching in a planar bipartite graph G . Then $f(G, M) = c(M)$, where $c(M)$ is the maximum number of disjoint M -alternating cycles of G .*

For a hexagon s in a hexagonal system H , the edges of s are denoted clockwise by e_1, e_2, e_3, f_1, f_2 and f_3 as shown in Figure 3 (sometimes we add superscript as $e_i^s, f_i^s, i = 1, 2, 3$). The hexagon s with perfect matchings $\{e_1, f_2, e_3\}$ and $\{f_1, e_2, f_3\}$ are *improper* and *proper* respectively (see Figure 3). A perfect matching M of H can be partitioned into three subsets, $E_1(M)$, $E_2(M)$ and $E_3(M)$, such that all edges in $E_i(M)$ are parallel to e_i (or f_i), $i = 1, 2, 3$.

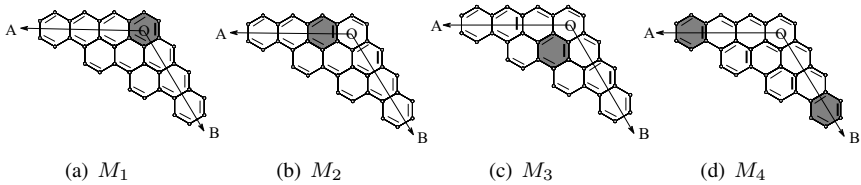

 Figure 3. A hexagon s with marked edges and two states.

Lemma 2.6. Let M be a perfect matching of a hexagonal system H . If $S \subset M$ can force an arbitrary edge subset $E_i(M)$, $i = 1, 2, 3$, then S is a forcing set of M .

Proof. Without loss of generality, assume S can force $E_1(M)$. Then $H \ominus S \subseteq H - V(E_1(M))$. Naturally, $M' =: E_2(M) \cup E_3(M)$ is a perfect matching of $H - V(E_1(M))$. Since any M -alternating cycle in H contains an edge in each $E_i(M)$ for $i = 1, 2, 3$, there is no M' -alternating cycles in $H - V(E_1(M))$. So $H - V(E_1(M))$ has a unique perfect matching M' . So $\emptyset$ is a forcing set of M' in $H - V(E_1(M))$. By Lemma 2.3, S can force M . $\square$

Let $T'(p)$ represent a *prolate triangle polyhex* with side length p , whose boundary faces consist of two linear hexagonal chains with length p and one zigzag hexagonal chain with length $2p - 1$ (see Figure 4). Let $T^r(p)$ represent a hexagonal system obtained from $T'(p)$ by adding r linear hexagonal chains with length p along one side (see Figure 5). Obviously, both $T'(p)$ and $T^r(p)$ are forced hexagonal systems. Zhang et al. [15] introduced an invariant triple (x, y, z) with $x \leq y \leq z$ for any perfect matching of a hexagonal system, where x, y and z are the numbers of double bonds of M in the three different directions and showed that x is an upper bound for the Clar number. Zhang [17] showed that the Clar numbers of $T'(p)$ and $T^r(p)$ are both equal to $x = p$. From [18, Theorem 4.5], we get the forcing spectra of $T'(p)$ and $T^r(p)$ are both continuous. For convenience, for integers $q \leq p$ we can use $[q, p]$ the integer interval consisting of all integers x with $q \leq x \leq p$.

Corollary 2.7 ([18]). $\text{Spec}(T'(p)) = [1, p]$.


 Figure 4. A perfect matching sequence $M_1M_2M_3M_4$ of $T'(4)$ and minimum forcing sets for each M_i .

Now we construct a perfect matching sequence $\{M_i\}_{i=1}^p$ of $T'(p)$ such that $f(T'(p), M_i) = i$. Let M_1 be the 3-divisible perfect matching of $T'(p)$ w.r.t. $O - ABC$. Let $H_i = \{s_{a,b,0} | a + b = i - 1\}$, $M_i = M_1 \triangle H_1 \triangle \cdots \triangle H_{i-1}$ and $S_i = \{e_2^s | s \in H_i\} = E_2(M_i)$ for $i = 1, 2, \dots, p$ (see Figure 4). Then S_i can force M_i by Lemma 2.6 and H_i consists of i disjoint M_i -alternating cycles, so $f(T'(p), M_i) = i$ by Lemma 2.5.

Corollary 2.8. $\text{Spec}(T^r(p)) = [1, p]$.

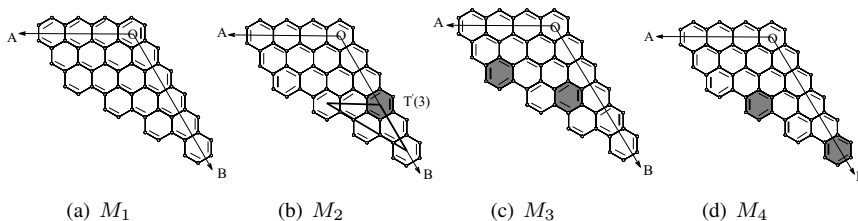


Figure 5. A perfect matching sequence $M_1 M_2 M_3 M_4$ of $T^2(4)$ and minimum forcing sets for each M_i .

Proof. For $T^r(p)$, we can construct a perfect matching sequence $\{M_i\}_{i=1}^p$ of $T^r(p)$ such that $f(T^r(p), M_i) = i$. Let M_1 be the 3-divisible perfect matching of $T^r(p)$ w.r.t. $O - ABC$. If $i \geq 2$, let M_i contain $f_2^{s_{p-1}, r, 0}$. As shown in Figure 5, $T^r(p) \ominus f_2^{s_{p-1}, r, 0}$ is isomorphic to $T'(p-1)$. Let $\{M'_i\}_{i=2}^{p-1}$ be a perfect matching sequence of $T'(p-1)$ such that $f(T'(p-1), M'_i) = i-1$. Let M_i be a perfect matching of $T^r(p)$ containing M'_i and $f_2^{s_{p-1}, r, 0}$. We can easily get $f(T^r(p), M_i) = i$. $\square$

3 Forcing spectra of convex hexagonal systems

Reference [17] found the expression of the Clar number of $O(m, k, n)$, which equals the maximum forcing number, and gave a construction for a Clar structure of $O(m, k, n)$, which plays an important role in our later proof.

Theorem 3.1 ([17]). *For any convex hexagonal system $O(m, k, n)$ ($m \leq k \leq n$) we have*

$$Cl(O(m, k, n)) = \begin{cases} mk - \frac{1}{4}\{(m+k-n)^2 - 1\}, & \text{if } m+k-n \geq 2 \text{ is odd,} \\ mk - \frac{1}{4}(m+k-n)^2, & \text{if } m+k-n \geq 2 \text{ is even,} \\ mk, & \text{if } m+k-n \leq 1. \end{cases}$$

Now we recall such construction for a Clar cover $C(r)$ of $O(m, k, n)$ (simply, H) with parameter r ($1 \leq r \leq m$) as follows (for details, see Proof (1) of Theorem 5 in [17]). Let $n_0 = \min\{n, m+k-r\}$. If $n_0 = n \leq m+k-r$, there exist six prolate triangle polyhexes on the corners of H respectively as $T_1 = T'(r)$, $T_2 = T'(k-r+1)$, $T_3 = T'(m-r+1)$, $T_4 = T'(n-k+r)$, $T_5 = T'(n-m+r)$, $T_6 = T'(m+k-n-r+1)$, and their maximum resonant sets are sequentially labeled $(s_1, s_2, \dots, s_r)$, $(s_r, s_{r+1}, \dots, s_k)$, $(h_1, \dots, h_{m-r+1})$, $(s_k, \dots, s_{n+r-1})$, $(h_{m-r+1}, \dots, h_n)$, $(h_n, \dots, h_{k+m-r})$, where $s_1 = h_1$ and $s_{n+r-1} = h_{k+m-r}$, and $s_1, s_r, s_k, h_{m-r+1}, s_{n+r-1}, h_n$ lie on the periphery of H (see Figure 6).

- (3) For each Clar cover $C_{m_0}(m_0)$ of H , there exists a perfect matching $M \in \mathcal{M}_{m_0}^{m_0}$ of H such that $f(H, M) = h(C_{m_0}(m_0)) + m - m_0$ for $1 \leq m_0 \leq m$.

Proof. (1) If $r \geq m + k - n$, let $M_r \in \mathcal{M}_r$ be a perfect matching of H such that $e_1^s \in M_r$ for any hexagon s in $C(r)$ and $S_r := \{e_1^s | s \in C(r)\}$ (see Figure 7). By Lemma 2.5 we have $f(H, M_r) \geq h(C(r)) = |S_r|$. As shown in Figure 7, we observe that $E_1(M_r) = S_r \cup (E(T_1) \cap E_1(M_r))$ and $S_r \cap E(T_1)$ can force $E(T_1) \cap E_1(M_r)$. So S_r can force $E_1(M_r)$. By Lemma 2.6 we have that S_r is a forcing set of M_r . So $f(H, M_r) = |S_r| = h(C(r))$.

If $r < m + k - n$, let $M_r \in \mathcal{M}_r$ be a perfect matching of H such that $e_1^s \in M_r$ for each hexagon $s \in F_i$ for $i > m - r$ and $f_1^s \in M_r$ for each hexagon $s \in F_i$ for $1 \leq i \leq m - r$ (see Figure 6). Let

$$S_r := \{e_1^s | s \in F_i, i > m - r\} \cup \{f_1^s | s \in F_i, 1 \leq i \leq m - r\}.$$

Similarly, it suffices to prove that S_r can force $E_1(M_r)$. As shown in Figure 6, we observe that $E_1(M_r) = S_r \cup (E(T_1) \cap E_1(M_r)) \cup (E(T_6) \cap E_1(M_r))$ and $S_r \cap E(T_1)$ can force $E(T_1) \cap E_1(M_r)$. Since $m - r + 1 \geq m + k - n - r + 1$, we can show that $S_r \cap E(T_6)$ can force $E(T_6) \cap E_1(M_r)$. So S_r can force $E_1(M_r)$.

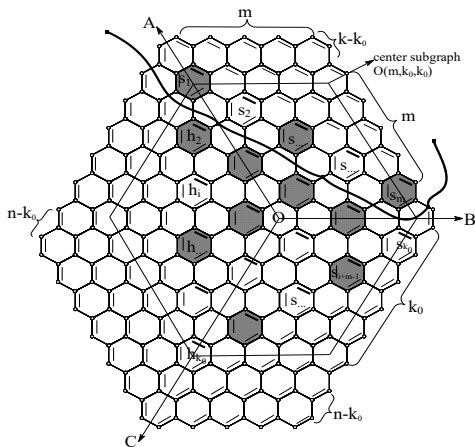


Figure 8. Clar cover $C_{m,k_0,k_0}(m)$ of H with perfect matching M .

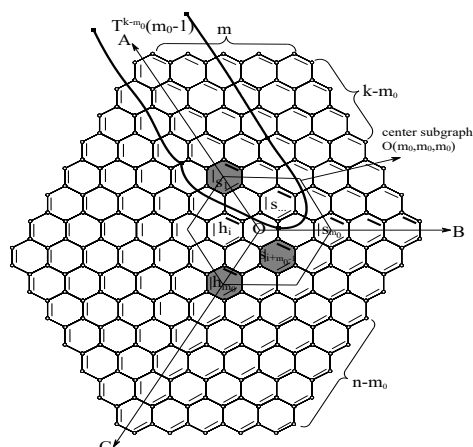


Figure 9. Clar cover $C_{m_0}(m_0)$ of H with perfect matching M .

(2) Let $M \in \mathcal{M}_{m,k_0,k_0}^{m,k_0,k_0}$ be a perfect matching of H such that $e_1^s \in M$ for each hexagon s in $C_{m,k_0,k_0}(m)$ and $S_{k_0} := \{e_1^s | s \in C_{m,k_0,k_0}(m)\}$ (see Figure 8). Similarly, it suffices to show that S_{k_0} can force $E_1(M)$. As shown in Figure 8, we observe that $E_1(M) = S_{k_0} \cup \{e_1^{s_{a,b,0}} : a + b \geq k_0\}$ and $S_{k_0} \cap \{e_1^{s_{a,b,0}} : a + b = k_0 - 1\}$ can force $\{e_1^{s_{a,b,0}} : a + b \geq k_0\}$. So S_{k_0} can force $E_1(M)$.

(3) Let $M \in \mathcal{M}_{m_0}^{m_0}$ be a perfect matching of H such that $e_1^s \in M$ for each hexagon s in $C_{m_0}(m_0)$ (see Figure 9). Let $L_{m_0} := \{e_1^{s_{0,m_0-1+i,0}} | 1 \leq i \leq m - m_0\}$ and $S_{m_0} := \{e_1^s | s \in C_{m_0}(m_0)\} \cup L_{m_0}$. As shown in Figure 9, we observe that the subgraph $H \ominus L_{m_0}$ is just $O(m_0, k, n)$. Since $O(m_0, m_0, m_0)$ is the center subgraph of $O(m_0, k, n)$, from (2) we know that $S_{m_0} \setminus L_{m_0}$ can force $M \cap E(O(m_0, k, n))$. By Proposition 2.4 we have that S_{m_0} is a forcing set of M . We can also get that there are $|S_{m_0}| - |L_{m_0}|$ disjoint

M -alternating hexagons in the center subgraph $O(m_0, k, n)$ (denoted by F'_{m_0}) which also belong to the center subgraph $O(m_0, m_0, m_0)$. As shown in Figure 11, the periphery of the center subgraph $O(m_0 + i, m_0 + i, m_0 + i)$ of H is an M -alternating cycle for all $i = 1, \dots, m - m_0$ and they do not intersect each other. Obviously these cycles do not intersect to each hexagon in F'_{m_0} . So $f(H, M_{m_0}^{m_0}) = |S_{m_0}| = h(C_{m_0}(m_0)) + m - m_0$. $\square$

References [21] and [14] have proved $f(O(m, k, n)) = m$ and $F(O(m, k, n)) = Cl(O(m, k, n))$ respectively. In the following, we divide the proof of our main theorem (see Theorem 3.6) into two parts: one is $[m, \frac{1}{2}m(m+1)] \subset \text{Spec}(H)$ (see Lemma 3.3); the other is $[\frac{1}{2}m(m+1), Cl(H)] \subseteq \text{Spec}(H)$ (see Corollary 3.5, which can be directly deduced from Lemma 3.4).

Lemma 3.3. *The integer interval $[m, \frac{1}{2}m(m+1)]$ is a subset of $\text{Spec}(H)$.*

Proof. By Theorem 3.2(3), there is $M_{m_0}^{m_0} \in \mathcal{M}_{m_0}^{m_0}$ such that $f(H, M_{m_0}^{m_0}) = h(C_{m_0}(m_0)) + m - m_0$ for $1 \leq m_0 \leq m$. So $f(H, M_1^1) = h(C_1(1)) + m - 1 = m$ and $f(H, M_m^m) = h(C_m(m)) = \frac{1}{2}m(m+1)$. It suffices to prove that $[f(H, M_{m_0-1}^{m_0-1}), f(H, M_{m_0}^{m_0})] \subseteq \text{Spec}(H)$ for $2 \leq m_0 \leq m$. Obviously $f(H, M_{m_0}^{m_0}) - f(H, M_{m_0-1}^{m_0-1}) = |C_0| = m_0 - 1$.

Let C be the set of all hexagons in $C_{m_0}(m_0)$. Let $C_0 := \{s_{a,b,0} | a+b = m_0 - 1, b \neq m_0 - 1\}$, $L_{m_0} := \{e_1^{s_0, m_0-1+i, 0} | 1 \leq i \leq m - m_0\}$ and $S_{m_0} := \{e_1^s | s \in C - C_0\} \cup L_{m_0}$.

Suppose $T^{k-m_0}(m_0 - 1)$ consists of hexagons $\{s_{a,b,0} | b \leq m_0 - 2, a+b \geq m_0 - 1\}$, as shown in Figure 9. We observe that $H \ominus S_{m_0} = T^{k-m_0}(m_0 - 1)$. By Corollary 2.8, we can get a perfect matching sequence $\{M'_j\}_{j=1}^{m_0-1}$ of $T^{k-m_0}(m_0 - 1)$ and the minimum forcing set S'_j for each M'_j such that $f(T^{k-m_0}(m_0 - 1), M'_j) = |S'_j| = j$. Let M_{m_0j} be a perfect matching of H obtained from $M_{m_0}^{m_0}$ by replacing the edges of $T^{k-m_0}(m_0 - 1)$ in $M_{m_0}^{m_0}$ with M'_j for all $j = 1, 2, \dots, m_0 - 1$. By Proposition 2.4, we know that $S_{m_0} \cup S'_j$ is a forcing set of M_{m_0j} .

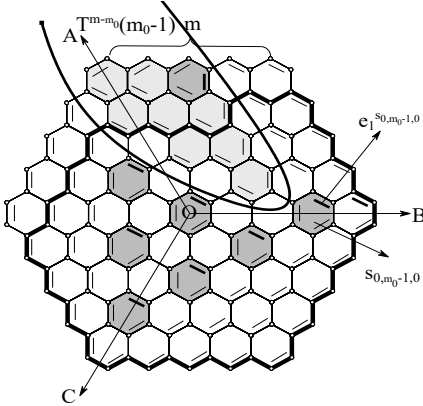


Figure 10. For $j = 1$, $|S_{m_0}| + |S'_1|$ disjoint M_{m_01} -alternating cycles.

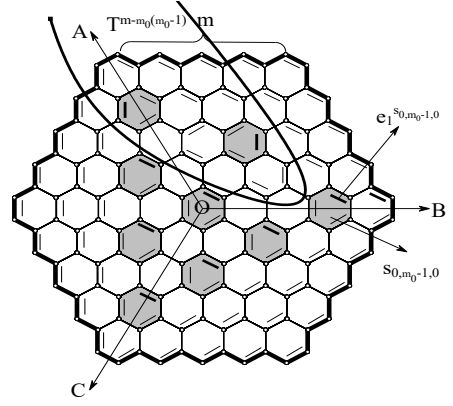


Figure 11. For $j \geq 2$, $|S_{m_0}| + |S'_1|$ disjoint M_{m_0j} -alternating cycles.

Next we shall prove that there exist $|S_{m_0}| + |S'_j|$ disjoint M_{m_0j} -alternating cycles in H . If it holds for $O(m, m, m)$, then it also holds for $O(m, k, n)$. From the structure of M_{m_0j} as above, we can find $|S_{m_0}| + |S'_j| - |L_{m_0}|$ disjoint M_{m_0j} -alternating hexagons in

H denoted by F'_j . Further it needs to find $m - m_0$ disjoint M_{m_0j} -alternating cycles not intersecting F'_j . If $j \geq 2$, as shown in Figure 11, we observe that the periphery of the center subgraph $O(m_0 + i, m_0 + i, m_0 + i)$ of H (denoted by C_{m_0+i}) is an $M_{m_0}^{m_0}$ -alternating cycle for $i = 1, \dots, m - m_0$. Because F'_j belongs to the center subgraph $O(m_0, m_0, m_0)$, F'_j and C_{m_0+i} do not intersect. So there exist $|S_{m_0}| + |S'_j|$ disjoint M_{m_0j} -alternating cycles for all $j = 2, \dots, m_0 - 1$. If $j = 1$, there also exist $|L_{m_0}|$ disjoint M_{m_01} -alternating cycles (see Figure 10), which do not intersect F'_1 . So there also exist $|S_{m_0}| + |S'_1|$ disjoint M_{m_01} -alternating cycles.

To sum up, for $1 \leq m_0 \leq m, 1 \leq j \leq m_0 - 1$ we have

$$f(H, M_{m_0j}) = |S_{m_0}| + |S'_j| = f(H, M_{m_0}^{m_0}) - (m_0 - 1) + j = f(H, M_{m_0-1}^{m_0-1}) + j.$$

So we get $[f(H, M_{m_0-1}^{m_0-1}), f(H, M_{m_0}^{m_0})] \subseteq \text{Spec}(H)$. $\square$

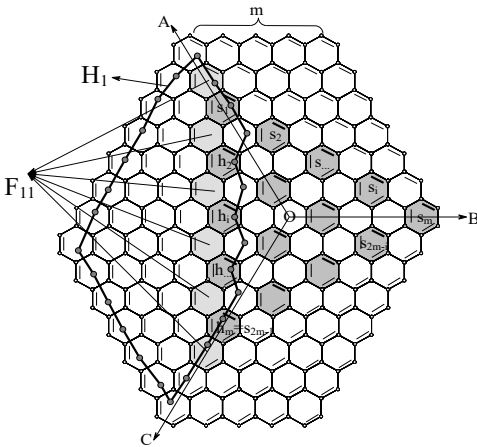


Figure 12. Clar cover $C_m(m)$ of H .

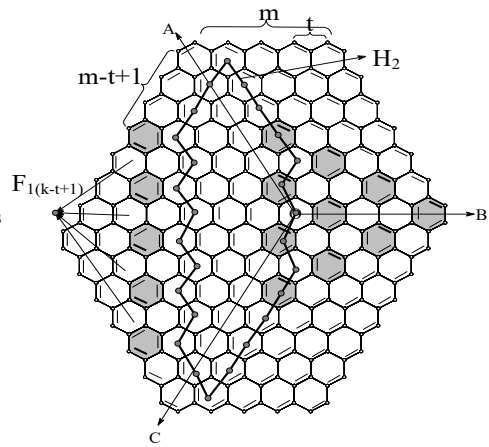


Figure 13. Perfect matching $M_{1(k-t+1)}$.

Among all Clar covers as $C(r)$ ($1 \leq r \leq m$) of H , we choose r as t such that $C(t)$ is a Clar structure of H , i.e. $h(C(t)) = Cl(H)$ is maximum.

From [17] we get that if $m - n + k \geq 2$, then $t = \lceil \frac{m-n+k+1}{2} \rceil$ or $\lfloor \frac{m-n+k+1}{2} \rfloor$; if $m - n + k \leq 1$ then $t = 1$. For example, for $O(5, 7, 8)$, $t = 2$ or 3 ; See Figure 6.

For the Clar cover $C_m(m)$ of H , recall the partition of the hexagons of $C_m(m)$ of H into m disjoint classes, where the i -th class, denoted by $\mathcal{F}_{i0}$ ($1 \leq i \leq m$), consists of hexagons lying on the i -th column left to right (see Figure 12).

Let $M_{10} \in \mathcal{M}_m^m$ be a perfect matching of H such that $e_1^s \in M$ for each hexagon s in $C_m(m)$ (each s is improper; see Figure 12). Next we define recursively a series of perfect matchings M_{1j} of H from M_{10} , $j = 1, 2, \dots, k - t + 1$. Let $M_{11} = M_{10} \triangle \mathcal{F}_{10}$. Then each hexagon of $\mathcal{F}_{10}$ becomes proper. This results in a series of new improper hexagons which are adjacent to hexagons of $\mathcal{F}_{10}$ via edges e_1 or e_3 . Let $\mathcal{F}_{11}$ be the set of such new improper M_{11} -alternating hexagons; In other words, $\mathcal{F}_{11}$ can be obtained from $\mathcal{F}_{10}$ by moving one column to the left (see Figure 12). Repeating the above procedure, let $M_{1j} = M_{1(j-1)} \triangle \mathcal{F}_{1(j-1)}$ for $j = 1, 2, \dots, k - t + 1$ and $\mathcal{F}_{1j}$ be the set of all improper M_{1j} -alternating hexagons minus all $M_{1(j-1)}$ -alternating hexagons; For example, see Figure 13 for $M_{1(k-t+1)}$.

For $i = 2, \dots, m, j \geq 1$, let $M_{ij} = M_{i0} \triangle \mathcal{F}_{i0} \triangle \dots \triangle \mathcal{F}_{i(j-1)}$, where $M_{i0} = M_{(i-1)(k-t+1)}$ or $M_{(i-1)(k-t)}$ according to $i \leq m-t+1$ or not, and $\mathcal{F}_{ij}$ is the set of improper M_{ij} -alternating hexagons minus all $M_{i(j-1)}$ -alternating hexagons. It is not difficult to find that $M_{m(k-t)} \in \mathcal{M}_t$ is a perfect matching of H corresponding to Clar structure $C(t)$, and $f(H, M_{m(k-t)}) = Cl(H)$. In this procedure if $i < m-t+1$, then $0 \leq j \leq k-t+1$ and we shift $\mathcal{F}_{i0}$ to the left $k-t+1$ times, else $0 \leq j \leq k-t$ and we shift it $k-t$ times (see Figures 6, 12 and 13).

From M_{10} to $M_{m(k-t)}$, we have already got a perfect matching sequence $M_{10}M_{11} \dots M_{1(k-t+1)} (= M_{20})M_{21} \dots M_{i0}M_{i1} \dots M_{m0} \dots M_{m(k-t)}$. Next we will prove that the difference of forcing numbers of two consecutive perfect matchings in this sequence is no more than 1.

Lemma 3.4. For $1 \leq i \leq m-t$ and $0 \leq j \leq k-t$, and $m-t+1 \leq i \leq m$ and $0 \leq j \leq k-t-1$, we have

$$|f(H, M_{i(j+1)}) - f(H, M_{ij})| \leq 1. \quad (3.1)$$

Proof. We recursively construct a minimum forcing set S_{ij} of M_{ij} so that $|S_{ij}|$ equals the maximum number of M_{ij} -alternating hexagons for $1 \leq i \leq m-t$ and $0 \leq j \leq k-t+1$, or $m-t+1 \leq i \leq m$ and $0 \leq j \leq k-t$.

For $i = 1, 0 \leq j \leq k-t+1$. Let $S'_1 := \{e_1^s | s \in \mathcal{F}_{i0}, 2 \leq i \leq m\}$. Then S'_1 can force $\{e_1^{s_{a,b,0}} | a+b \geq m-1, b \geq 1\}$ (see Figure 12) and $H_1 := H \ominus S'_1$ is shown in Figure 14. If $n-m+1 < k-t+1$ (in this case T_6 in $C(t)$ has length $m+k-n-t+1 \geq 2$ and $\mathcal{F}_{1(k-t)}$ lies on the area AOC ; see Figures 13 and 14), let

$$S'_{1j} = \begin{cases} \{e_1^s | s \in \mathcal{F}_{1j}\}, & \text{if } 0 \leq j \leq n-m, \\ \{f_1^s | s \in \mathcal{F}_{1(j-1)}\}, & \text{if } n-m+1 \leq j \leq k-t+1. \end{cases}$$

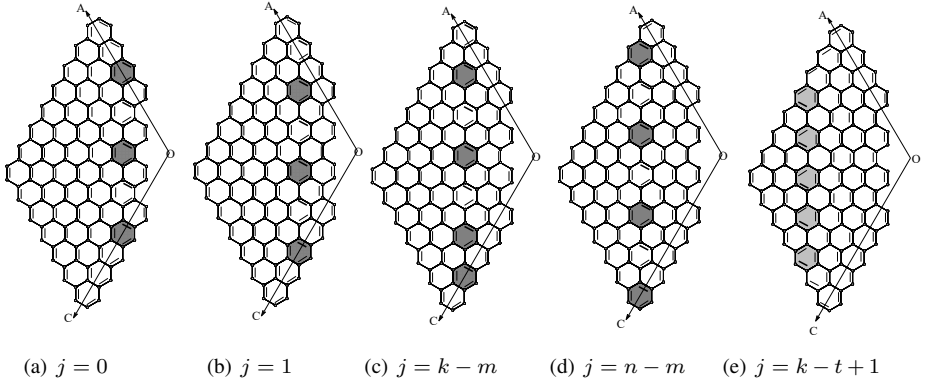


Figure 14. Illustration for $M_{1j} \cap E(H_1)$ and S'_{1j} with $j = 0, 1, k-m, n-m, k-t+1$.

Since S'_{1j} can force $E(H_1) \cap E_1(M_{1j})$ (see Figure 14), $S_{1j} := S'_1 \cup S'_{1j}$ can force $E_1(M_{1j})$ by Proposition 2.4. Further we get that S_{1j} is a forcing set of M_{1j} by Proposition 2.6.

On the other hand, there exist $|S_{1j}|$ disjoint M_{1j} -alternating hexagons of H , so S_{1j} is a minimum forcing set of M_{1j} and

$$f(H, M_{1j}) = |S_{1j}| = \begin{cases} |\mathcal{F}_{1j}| + |S'_1|, & \text{if } 0 \leq j \leq n - m, \\ |\mathcal{F}_{1(j-1)}| + |S'_1|, & \text{if } n - m + 1 \leq j \leq k - t + 1. \end{cases} \quad (3.2)$$

Combining Equation (3.2) we can get

$$f(H, M_{1(j+1)}) - f(H, M_{1j}) = \begin{cases} |\mathcal{F}_{1(j+1)}| - |\mathcal{F}_{1j}| = 1, & \text{if } 0 \leq j \leq k - m - 1, \\ |\mathcal{F}_{1(j+1)}| - |\mathcal{F}_{1j}| = 0, & \text{if } k - m \leq j \\ & \leq n - m - 1 (k < n), \\ |\mathcal{F}_{1j}| - |\mathcal{F}_{1j}| = 0, & \text{if } j = n - m, \\ |\mathcal{F}_{1j}| - |\mathcal{F}_{1(j-1)}| = -1, & \text{if } n - m + 1 \leq j \leq k - t. \end{cases}$$

Otherwise, $n - m + 1 \geq k - t + 1$ (see Figures 15 and 16), let

$$S'_{1j} = \{e_1^s | s \in \mathcal{F}_{1j}, 0 \leq j \leq k - t + 1\}.$$

Then $S_{1j} = S'_1 \cup S'_{1j}$ can force $E_1(M_{1j})$. Similarly we have that S_{1j} is a minimum forcing set of M_{1j} . So

$$f(H, M_{1(j+1)}) - f(H, M_{1j}) = \begin{cases} |\mathcal{F}_{1(j+1)}| - |\mathcal{F}_{1j}| = 1, & \text{if } 0 \leq j \leq k - m - 1, \\ |\mathcal{F}_{1(j+1)}| - |\mathcal{F}_{1j}| = 0, & \text{if } k - m \leq j \leq k - t. \end{cases}$$

To sum up, the lemma is true for $i = 1$.

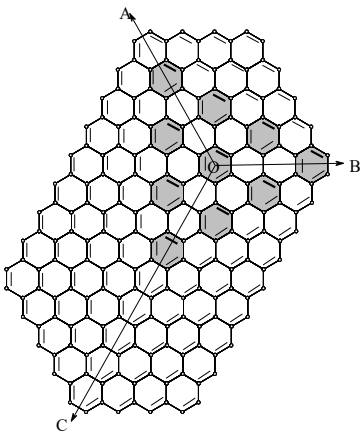


Figure 15. Perfect matching M_{10} .

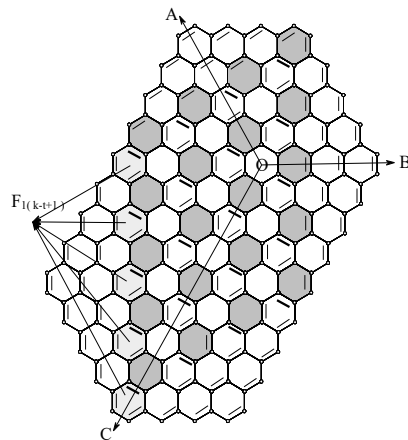


Figure 16. Perfect matching $M_{m(k-t)}$ and $\mathcal{F}_{1(k-t+1)}$ with $n - m + i \geq k - t + 1$.

For $2 \leq i \leq m$, suppose that a minimum forcing set $S_{(i-1)j}$ of $M_{(i-1)j}$ has been already given. Next we construct a minimum forcing set S_{ij} of M_{ij} from S_{i0} , which is identical to $S_{(i-1)(k-t+1)}$ or $S_{(i-1)(k-t)}$ according to $i < m - t + 1$ or not.

For $i < m - t + 1$, we have $0 \leq j \leq k - t + 1$. Let $S_{ij} = S'_i \cup S'_{ij}$, where $S'_i = S_{(i-1)(k-t+1)} - \{e_1^s | s \in \mathcal{F}_{i0}\}$ and S'_{ij} will be given next. If $n - m + i < k - t + 1$, let

$$S'_{ij} = \begin{cases} \{e_1^s | s \in \mathcal{F}_{ij}\}, & \text{if } 0 \leq j \leq n - m + i - 1, \\ \{f_1^s | s \in \mathcal{F}_{i(j-1)}\}, & \text{if } n - m + i \leq j \leq k - t + 1 \end{cases}$$

else

$$S'_{ij} = \{e_1^s | s \in \mathcal{F}_{ij}, 0 \leq j \leq k - t + 1\}.$$

For such perfect matching M_{ij} of H , let $H_i := H \ominus S'_i$; For example, H_2 is shown in Figures 13 and 18 (it consists of hexagons on the closed broken segment and its interior). For $n - m + i < k - t + 1$, if $0 \leq j \leq k - m + i - 2$, as shown in Figure 17 and Figure 18 (a)-(b), we observe that $E(H_i) \cap E_1(M_{ij}) - S'_{ij}$ appears on a linear hexagonal chain $\{s_{a,i-1,0} | m - i + j + 1 \leq a \leq k - 1\}$ along the shifts of $s_{m-i,i-1,0}$, and $e_1^{s_{m-i+j,i-1,0}}$ can force $E(H_i) \cap E_1(M_{ij}) - S'_{ij}$. So S'_{ij} can force $E(H_i) \cap E_1(M_{ij})$; If $k - m + i - 1 \leq j \leq n - m + i$, as shown in Figure 18 (b) and (c) we observe that $S'_{ij} = E(H_i) \cap E_1(M_{ij})$, and S'_{ij} can force $E(H_i) \cap E_1(M_{ij})$; if $n - m + i + 1 \leq j \leq k - t + 1$, then as shown in Figures 17 and 18(d), we observe that $E(H_i) \cap E_1(M_{ij}) - S'_{ij}$ appears on a linear hexagonal chain

$$\{s_{a,0,n-i} | 0 \leq a \leq j - 1 - (n - m + i + i - 1)\} \cup \{s_{0,b,n-i} | i - 1 - (j - 1 - (n - m + i)) \leq b \leq i - 1\}$$

along the shifts of hexagon $s_{0,i-1,m-i}$, and $f_1^{s_{j-(n-m+2i-1),0,n-i}}$ or $f_1^{s_{0,i-1-j+(n-m+i),n-i}}$ can force $E(H_i) \cap E_1(M_{ij}) - S'_{ij}$. So S'_{ij} can force $E(H_i) \cap E_1(M_{ij})$. For $n - m + i + 1 \geq k - t + 1$, similarly S'_{ij} can force $E(H_i) \cap E_1(M_{ij})$. By Proposition 2.4, we know that S_{ij} is a forcing set of M_{ij} . On the other hand there also exist $|S_{ij}|$ disjoint M_{ij} -alternating hexagons of H . Then S_{ij} is the minimum forcing set of M_{ij} i.e.

$$f(H, M_{ij}) = |S_{ij}| = \begin{cases} |\mathcal{F}_{ij}| + |S'_i|, & \text{if } 0 \leq j \leq n - m + i - 1, \\ |\mathcal{F}_{i(j-1)}| + |S'_i|, & \text{if } n - m + i \leq j \leq k - t + 1. \end{cases} \quad (3.3)$$

So, if $n - m + i < k - t + 1$, combining Equation (3.3) we get

$$f(H, M_{i(j+1)}) - f(H, M_{ij}) = \begin{cases} |\mathcal{F}_{i(j+1)}| - |\mathcal{F}_{ij}| = 1, & \text{if } 0 \leq j \leq k - m + i - 2, \\ |\mathcal{F}_{i(j+1)}| - |\mathcal{F}_{ij}| = 0, & \text{if } k - m + i - 1 \leq j \\ & \leq n - m + i - 2 (k < n), \\ |\mathcal{F}_{ij}| - |\mathcal{F}_{ij}| = 0, & \text{if } j = n - m + i - 1, \\ |\mathcal{F}_{ij}| - |\mathcal{F}_{i(j-1)}| = -1, & \text{if } n - m + i \leq j \leq k - t; \end{cases}$$

else

$$f(H, M_{i(j+1)}) - f(H, M_{ij}) = \begin{cases} |\mathcal{F}_{i(j+1)}| - |\mathcal{F}_{ij}| = 1, & \text{if } 0 \leq j \leq k - m + i - 2, \\ |\mathcal{F}_{i(j+1)}| - |\mathcal{F}_{ij}| = 0, & \text{if } k - m + i - 1 \leq j \leq k - t. \end{cases}$$

The remaining case is $i \geq m - t + 1$. Then $0 \leq j \leq k - t$. Let $S'_i = S_{(i-1)(k-t)} - \{e_1^s | s \in \mathcal{F}_{i0}\}$ and $S'_{ij} = \{e_1^s | s \in \mathcal{F}_{ij} | 0 \leq j \leq k - t\}$. Similarly S_{ij} is a minimum forcing set of M_{ij} . So $f(H, M_{i(j+1)}) - f(H, M_{ij}) = 1$ for all $j = 0, 1, 2, \dots, (k - t - 1)$. The proof is complete. $\square$

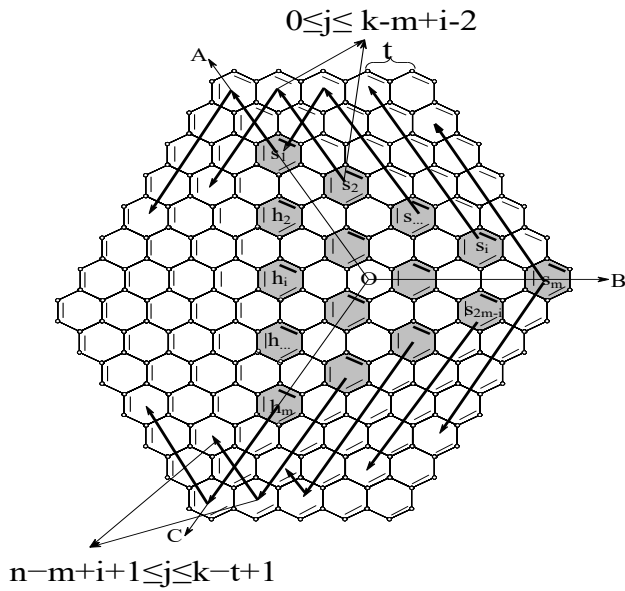


Figure 17. j shifts of hexagons $s_{m-i, i-1, 0}$ and $s_{0, i-1, m-i}$ for $i = 1, 2, \dots, m$.

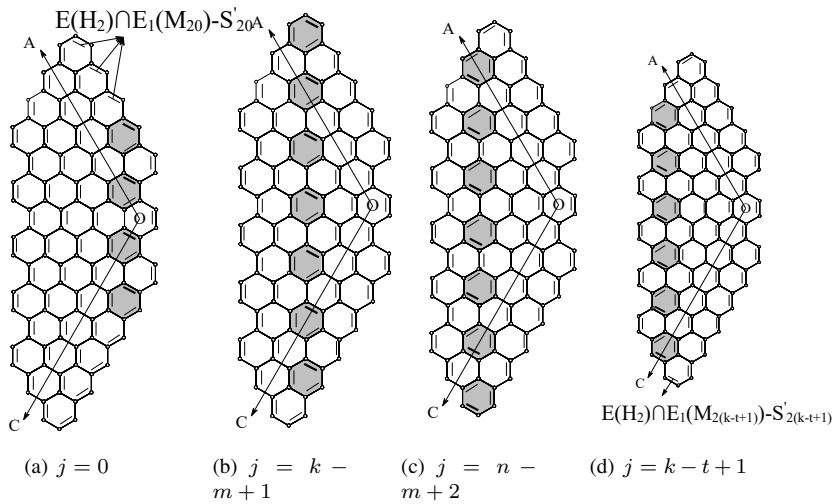


Figure 18. Illustration for $M_{2j} \cap E(H_2)$ and S'_{2j} with $j = 0, k-m+1, n-m+2, k-t+1$.

By Theorem 3.2, we get $f(H, M_{10}) = \frac{1}{2}m(m+1)$ and $f(H, M_{m(k-t)}) = Cl(H)$. As an immediate consequence of Lemma 3.4, we obtain the following result.

Corollary 3.5. *The integer interval $[\frac{1}{2}m(m+1), Cl(O(m, k, n))]$ is a subset of $\text{Spec}(H)$.*

By Lemma 3.3 and Corollary 3.5 we get the following main result.

Theorem 3.6. *For any convex hexagonal systems $O(m, k, n)$, then $\text{Spec}(O(m, k, n)) = [m, Cl(O(m, k, n))]$.*

Remark 3.1. The method in obtaining Lemma 3.4 and Corollary 3.5 can be used to discuss the forcing spectra of other types of hexagonal systems. There is an alternative approach to obtain Corollary 3.5 as follows. Similar to the proof of Lemma 3.3, from the Clar covers $C(r)$ of $O(m, k, n)$ for $r \in [t, m]$, where $C(t)$ is a Clar structure, we can construct a series of perfect matchings to show that $[\frac{1}{2}m(2k+1-m), Cl(O(m, k, n))] \subset \text{Spec}(O(m, k, n))$, and from the Clar covers $C_{m, k_0, k_0}(m)$ of $O(m, k, n)$ for $k_0 \in [m, k]$, we can construct a series of perfect matchings to show that $[\frac{1}{2}m(m+1), \frac{1}{2}m(2k+1-m)] \subset \text{Spec}(O(m, k, n))$.

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