ISSN 1855-3966 (printed edn.), ISSN 1855-3974 (electronic edn.)
ARS MATHEMATICA CONTEMPORANEA 15 (2018) 191–204
https://doi.org/10.26493/1855-3974.1279.bce
(Also available at http://amc-journal.eu)

Saturation number of lattice animals

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Received 7 January 2017, accepted 24 October 2017, published online 19 June 2018

Abstract

A matching M in a graph G is maximal if no other matching of G has M as a proper subset. The saturation number of G is the cardinality of any smallest maximal matching in G. In this paper we investigate saturation number for several classes of square and hexagonal lattice animals.

Keywords: Maximal matching, saturation number, lattice animal, polyomino graph, benzenoid graph, coronene.

Math. Subj. Class.: 92E10, 05C70, 05C35, 05C90

*Partially supported by the Croatian Science Foundation via research projects BioAmpMode (Grant no. 8481) and LightMol (Grant no. IP-2016-06-1142) and by Croatian Ministry of Science, Education and Sports (Croatian-Slovenian bilateral project "*Modeling adsorption on nanostructures: Graph-theoretic approach*").

†Supported by the Slovenian Research Agency.

‡Supported in part by the Slovenian Research Agency under grant P1-0297.

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1 Introduction

A lattice animal is any bounded subset of a regular lattice in the plane whose boundary is made of simple closed curve following lattice edges. In this paper we study the saturation number of hexagonal and square lattice animals.

The saturation number $s(G)$ of a graph G is the cardinality of a smallest maximal matching in G. Maximal matchings serve as models of adsorption of dimers (those that occupy two adjacent atoms) to a molecule. It can occur that the bonds in a molecule are not efficiently saturated by dimers, and therefore, their number is below the theoretical maximum. Hence, the saturation number provides an information on the worst possible case of adsorption. Besides in chemistry the saturation number has a number of interesting applications in engineering and networks. The problem of determining the saturation number is equivalent to the problem of finding the edge domination number in a graph. Moreover, if a graph G has an efficient edge dominating set D, it holds $s(G) = |D|$ (see [7]). Previous work on the saturation number includes research on random graphs [8, 9], on benzenoid systems [5], fullerenes [1, 2, 4], and nanotubes [7]. Recent results on related concepts can be found in [3, 6].

2 Preliminaries

A *matching* M in a graph G is a set of edges of G such that no two edges from M share a vertex. A matching M is a *maximum matching* if there is no matching in G with greater cardinality. The cardinality of any maximum matching in G is denoted by $\nu(G)$ and called the *matching number* of G. If every vertex of G is incident with an edge of M, the matching M is called a *perfect matching* (in chemistry perfect matchings are known as *Kekulé structures*).

A matching M in a graph G is *maximal* if it cannot be extended to a larger matching in G. Obviously, every maximum matching is also maximal, but the opposite is generally not true. A matching M is a *smallest maximal matching* if there is no maximal matching in G with smaller cardinality. The cardinality of any smallest maximal matching in G is the *saturation number* of G, denoted by $s(G)$.

The following lemma is very useful for proving lower bounds for the saturation number. The proof can be found in [7]. See also [8, 9].

Lemma 2.1. *Let G be a graph and let A and B be maximal matchings in G. Then $|A| \geq \frac{|B|}{2}$ and $|B| \geq \frac{|A|}{2}$.*

This result implies the lower bound $s(G) \geq \frac{\nu(G)}{2}$. In particular, in graphs with perfect matchings the saturation number cannot be smaller than one quarter of the number of vertices, $s(G) \geq \frac{n}{4}$.

A *polyomino system* consists of a cycle C in the infinite square lattice together with all squares inside C. A *polyomino graph* is the underlying graph of a polyomino system.

A *benzenoid system* consists of a cycle C in the regular infinite hexagonal lattice together with all hexagons inside C. A *benzenoid graph* is the underlying graph of a benzenoid system.

Let G be a benzenoid graph or a polyomino graph. The vertices lying on the outer face of G are called *external*; other vertices, if any, are called *internal*. Graph G without internal vertices is called *catacondensed*. If no inner face in a catacondensed graph G is adjacent to more than two other inner faces, we say that graph G is *unbranched* or that it is a *chain*.

In each chain G there are exactly two inner faces adjacent to one other inner face; those two inner faces are called *terminal*, while any other inner faces are called *interior*. The number of inner faces in chain G is called its *length*. An interior inner face is called *straight* if the two edges it shares with other inner faces are parallel, i.e. opposite to each other. If the shared edges are not parallel, the inner face is called *kinky*. If all interior inner faces of a chain G are straight, the chain is called *linear*.

There is also another terminology, calling straight inner faces *linear*, and kinky inner faces *angular*. By introducing abbreviations L and A, respectively, for linear and angular inner faces, each chain can be represented as a word over the alphabet $\{L, A\}$, with the restriction that the first and the last letter are always L. Such a word is called the LA-sequence of the chain.

A *fullerene* F is a 3-connected 3-regular plane graph such that every face is bounded by either a pentagon or a hexagon. By Euler's formula, it follows that the number of pentagonal faces of a fullerene is exactly 12.

The *Cartesian product* $G \,\square\, H$ of graphs G and H is the graph with the vertex set $V(G) \times V(H)$ and $(a, x)(b, y) \in E(G \,\square\, H)$ whenever $ab \in E(G)$ and $x = y$, or, if $a = b$ and $xy \in E(H)$.

3 Polyomino chains and grid graphs

In this section we prove some results regarding the saturation number of polyomino chains and rectangular grids. We start with the linear chain L_n, where n denotes the number of squares. Such chain can be obtained as Cartesian product of the path P_n of length n and K_2. Here P_n is the path on n edges so that $L_n = P_n \,\square\, K_2$. Alternatively, $L_n = P_n \,\square\, P_1$. We draw L_n so that the edges of both copies of P_n are horizontal, see Figure 1.

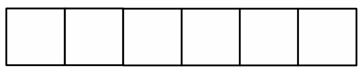

Figure 1: Linear polyomino chain $L_6 = P_6 \,\square\, K_2$.

We start by quoting two facts about the saturation number and the structure of smallest matchings in paths.

Proposition 3.1 ([6]). *Let P_n be a path of length n. Then $s(P_n) = \lceil \frac{n}{3} \rceil$. More precisely,*

$$s(P_n) = \begin{cases} \frac{n}{3}, & 3 \mid n \\ \frac{n+2}{3}, & 3 \mid (n-1) \\ \frac{n+1}{3}, & 3 \mid (n-2). \end{cases}$$

Proposition 3.2. *Let P_n be a path of length n. Then P_n has a smallest maximal matching that leaves at least one of the end-vertices unsaturated.*

Proof. Let n be divisible by 3. We form groups of three consecutive edges and construct a matching M by taking the middle edge of each group. M is obviously a smallest maximal matching and leaves unsaturated both end-vertices of P_n. If $n = 3k + 1$, again consider groups of 3 consecutive edges, take the middle edge in each group and add the sole edge that does not belong to any group. Again the constructed matching is a smallest maximal matching. Finally, when $n = 3k + 2$, construct a matching in the same way by taking the middle edge from each of k groups of three consecutive edges and adding the edge saturating the rightmost vertex. □

Next we show that we can construct a smallest maximal matching in L_n without using vertical edges. This result will enable us to reduce the problem of finding the saturation number of L_n to known results about $s(P_n)$.

Proposition 3.3. *Let M be a maximal matching in L_n containing $k > 0$ vertical edges. Then there is another maximal matching M' in L_n containing $k' < k$ vertical edges such that $|M'| \leq |M|$.*

Proof. We label the vertices in the upper copy of P_n with $u_0, u_1, \dots, u_n$, from left to right, and vertices in the lower copy with $v_0, v_1, \dots, v_n$, in the same direction. There are $n + 1$ vertical edges, each of the form $u_i v_i$ for some $0 \leq i \leq n$. See Figure 2.

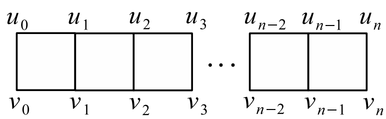

Figure 2: Linear polyomino chain L_n.

Let M be a maximal matching in L_n with $k > 0$ vertical edges and let the leftmost vertical edge in M be the edge $u_m v_m$. Obviously, m cannot be equal to 1.

We consider first the case $m = 0$. If $u_1 v_1$ is also in M, we construct a matching M' as $M' = M - \{u_0 v_0, u_1 v_1\} \cup \{u_0 u_1, v_0 v_1\}$. Obviously, M' is a maximal matching of the same cardinality as M containing $k - 2$ vertical edges.

Let now both neighbors u_1 and v_1 of end-vertices of $u_0 v_0$ be saturated by horizontal edges. Hence, both $u_1 u_2$ and $v_1 v_2$ are in M. Then at least one of u_3 and v_3 must be saturated by an edge of M. Let u_3 be saturated. Then we can construct a matching M' as $M' = M - \{u_0 v_0, u_1 u_2\} \cup \{u_0 u_1\}$. Again, M' is a maximal matching, $|M'| = |M| - 1$ and $k' = k - 1$. The case of saturated v_3 follows by symmetry.

The last case to consider for $m = 0$ is the one in which only one of u_1, v_1 is saturated by a, necessarily horizontal, edge of M. Let it be u_1. Hence, $u_1 u_2 \in M$ and $v_1 v_2 \notin M$. Then v_3 must be saturated and $M' = M - \{u_0 v_0\} \cup \{v_0 v_1\}$ is a maximal matching of the same cardinality as M but with one vertical edge less. Hence, the claim holds if the leftmost vertical edge in M is $u_0 v_0$. This case is depicted in Figure 3.

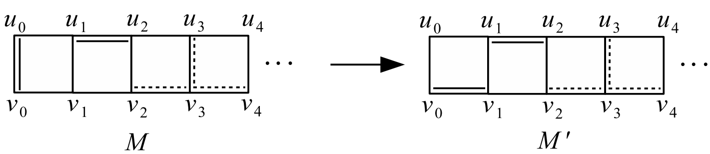

Figure 3: The case when $m = 0$ and only one of u_1,v_1 is saturated by M.

Let now the leftmost vertical edge in M be $u_2 v_2$. Then both $u_0 u_1$ and $v_0 v_1$ must be in M, and at least one of vertices u_3 and v_3 must be saturated by an edge of M. Let it be

u_3. Then the matching M' constructed as $M' = M - \{u_2v_2, v_0v_1\} \cup \{v_1v_2\}$ will be a maximal matching with smaller cardinality and with one vertical edge less than M.

Similar constructions apply when the leftmost vertical edge of M is near the right end of the chain. The simplest is the case $m = n - 1$, when also the rightmost edge u_nv_n must be in M. Then by switching the edges on the rightmost square one readily obtains a maximal matching of the same size as M but without vertical edges. The case $m = n - 2$ forces both horizontal edges $u_{n-1}u_n$ and $v_{n-1}v_n$ to be in M. Then at least one of u_{n-3} and v_{n-3} must be saturated. Let it be v_{n-3}. Then the matching $M' = M - \{u_{n-2}v_{n-2}, u_{n-1}u_n\} \cup \{u_{n-2}u_{n-1}\}$ is a maximal matching of smaller size than M without vertical edges. Remains the case when u_nv_n is the leftmost (and hence the only) vertical edge in M. If only one of u_{n-1}, v_{n-1} is saturated, let us say u_{n-1}, it suffices to switch u_nv_n and $v_{n-1}v_n$ to obtain a maximal matching M' of the same size without vertical edges. If both u_{n-1}, v_{n-1} are saturated, they must be saturated by horizontal edges $u_{n-2}u_{n-1}$ and $v_{n-2}v_{n-1}$, respectively. Also, at least one of u_{n-3} and v_{n-3} must be saturated. Let it be v_{n-3}. Then $M' = M - \{u_nv_n, v_{n-2}v_{n-1}\} \cup \{v_{n-1}v_n\}$ is a maximal matching of smaller size than M but without vertical edges.

Now we can look at the remaining cases in a unified manner. So, let u_mv_m, $3 \leq m \leq n-3$, be the leftmost vertical edge in a maximal matching M. If $u_{m+1}v_{m+1}$ is also in M, we construct M' by switching the edges on the square $u_m, u_{m+1}, v_{m+1}, v_m$, obtaining a maximal matching of the same size but with two vertical edges less. Hence, we can suppose that $u_{m+1}v_{m+1} \notin M$.

If both u_{m-1} and u_{m+1} are unsaturated, then both v_{m-1} and v_{m+1} must be saturated, necessarily by horizontal edges $v_{m-2}v_{m-1}$ and $v_{m+1}v_{m+2}$, respectively. Further, both u_{m-2} and u_{m+2} must be saturated, again by horizontal edges. The situation is shown in Figure 4.

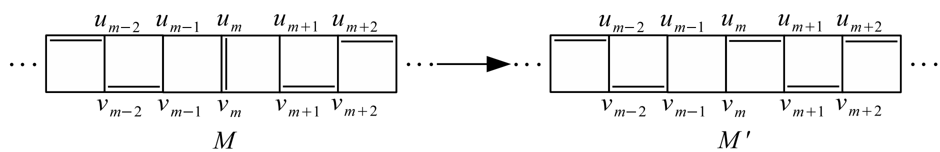

Figure 4: The case when u_{m-1} and u_{m+1} are both unsaturated.

We construct M' as $M' = M - \{u_mv_m\} \cup \{u_mu_{m+1}\}$. Obviously, M' is a maximal matching of the same size as M and with one vertical edge less. The situation in which both v_{m-1} and v_{m+1} are unsaturated follows by symmetry.

It remains to consider the case when at least one of u_{m-1}, u_{m+1} and at least one of v_{m-1}, v_{m+1} are saturated. We construct a new matching M'' by keeping the part of M to the left of u_mv_m, shifting all edges of M that were right of u_mv_m one place to the left (hence, u_lu_{l+1} goes to $u_{l-1}u_l$, v_lv_{l+1} to $v_{l-1}v_l$ and u_lv_l to $u_{l-1}v_{l-1}$ for $m < l \leq n$) and moving u_mv_m to u_nv_n. Obviously, M'' is a maximal matching of the same size as M and with the same number of vertical edges, but with the leftmost vertical edge at some place $l > m$. Let us look at the situation on the right-hand side of L_n.

If $u_{n-1}v_{n-1}$ is in M'', then M' with the desired properties can be obtained by switching edges on the rightmost square of L_n. If $u_{n-1}v_{n-1}$ is not in M'', then also $u_{n-2}v_{n-2}$ cannot be in M, and M' can be constructed in exactly the same manner as when u_nv_n is the only vertical edge in M.

Hence, no matter where in M the leftmost vertical edge appears, we can always construct a maximal matching of the same or smaller size with strictly smaller number of vertical edges. $\square$

Corollary 3.4. *There is a maximal matching in L_n of cardinality $s(L_n)$ without vertical edges.*

Corollary 3.5. $2s(P_n) \leq s(L_n) \leq 2s(P_n) + 1$.

Proof. We know that there is a smallest maximal matching M in L_n (i.e., of the size equal to $s(L_n)$) without vertical edges. Hence all edges of M are horizontal, and each edge belongs to one of two copies of P_n in L_n. If the cardinality of M is smaller than $2s(P_n)$, then at least one of two copies of P_n will contain two adjacent unsaturated vertices. This proves the left inequality.

To prove the right inequality, let us take a smallest maximal matching M_u in the upper copy of P_n. If M_u saturates exactly one end-vertex of P_n, let us take it so that it saturates u_0. Let M_v be a smallest maximal matching in the lower copy of P_n obtained by taking the edges corresponding to the edges of M_u and shifting them one place to the right. Then M_v saturates the vertices in the lower copy of P_n adjacent to the vertices of the upper copy of P_n left unsaturated by M_u. Hence $M = M_u \cup M_v$ is a maximal matching in L_n of size $2s(P_n)$.

It remains to consider the case when all smallest maximal matchings in P_n leave both end-vertices unsaturated. In that case, take two smallest maximal matchings M_u and M_v in upper and lower copy of P_n, respectively, and shift M_v one place to the right so that it saturates the neighbors of the vertices left unsaturated by M_u. That leaves unsaturated both end-vertices of v_0v_1. By adding that edge to the maximal matching constructed from M_u and shifted M_v we obtain a maximal matching of size $2s(P_n) + 1$. $\square$

From this we can get the exact expression for the saturation number of the linear polyomino chain.

Theorem 3.6. *Let L_n be the linear polyomino chain. Then*

$$s(L_n) = \begin{cases} \frac{2n}{3} + 1, & 3 \mid n \\ \frac{2(n+2)}{3}, & 3 \mid (n-1) \\ \frac{2(n+1)}{3}, & 3 \mid (n-2). \end{cases}$$

Proof. If $3 \mid (n-1)$ or $3 \mid (n-2)$ there is a smallest maximal matching M for P_n such that M saturates exactly one end-vertex of P_n. Therefore, it follows from the proof of Corollary 3.5 that $s(L_n) = 2s(P_n)$ and we are done. If $3 \mid n$, the smallest maximal matching of P_n is uniquely defined and it leaves both end-vertices unsaturated. Hence, in this case we obtain $s(L_n) > 2s(P_n)$ and therefore, $s(L_n) = 2s(P_n) + 1$.

Examples of smallest maximal matchings in L_n for all classes of divisibility of the chain length by 3 are given in the Figure 5. $\square$

The above approach can be successfully applied also to obtain non-trivial upper bounds on the saturation number of grid graphs that arise as Cartesian products of two (or more) paths. By taking smallest maximal matchings in all horizontal (or in all vertical) copies of paths in $P_m \,\square\, P_n$, shifting them and adjusting by adding an edge where necessary, and using symmetry, we can obtain following upper bound on $s(P_m \,\square\, P_n)$.

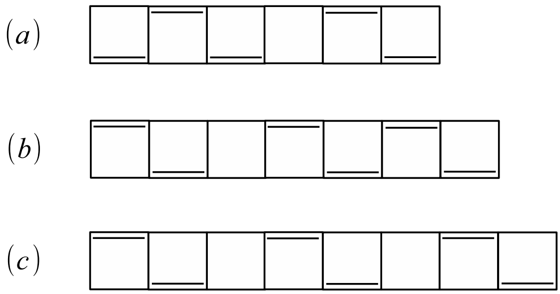

Figure 5: Linear polyomino chains with maximal matchings.

Proposition 3.7. $s(P_m \,\square\, P_n) \leq \min\{(m+1)[s(P_n)+1], (n+1)[s(P_m)+1]\}$.

This upper bound can be improved a bit by exploiting particular relationships between parities and remainders modulo 3 of m and n. See Figure 6 for an example. We believe, however, that our upper bounds capture the asymptotic behavior of the saturation number of rectangular grids.

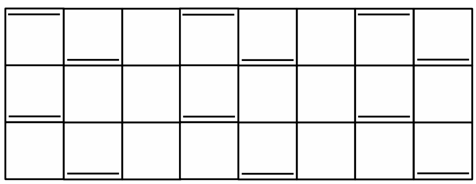

Figure 6: Graph $P_8 \,\square\, P_3$ with a maximal matching.

Now we go back to polyomino chains. In the following theorem we give the exact closed formulas for the saturation number of polyomino chains where all internal squares are kinky.

Theorem 3.8. *Let S_k be a polyomino chain with k squares such that all internal squares are kinky. Then*

$$s(S_k) = \left\lceil \frac{k}{2} \right\rceil + 1.$$

Proof. We consider two cases.

1. Let k be even. Since the number of vertices in S_k is $2k+2$, a perfect matching (which always exists) has $k+1$ edges. Using Lemma 2.1 we obtain that $s(S_k) \geq \frac{k+1}{2}$. Since k is even, we obtain $s(S_k) \geq \lceil \frac{k}{2} \rceil + 1$. To show the upper bound, we construct a maximal matching M from Figure 7.

   Obviously, $|M| = \frac{k}{2} + 1 = \lceil \frac{k}{2} \rceil + 1$. Hence, $s(S_k) = \lceil \frac{k}{2} \rceil + 1$.

2. If k is odd, let M' be a maximal matching from Figure 8.

   Obviously, $|M'| = \frac{k+1}{2} + 1$ and therefore, $s(S_k) \leq \frac{k+1}{2} + 1 = \lceil \frac{k}{2} \rceil + 1$. Now suppose that there is a maximal matching N for S_k such that $|N| \leq \frac{k+1}{2}$. It is easy to see that at least one of edges e_1, e_2, and e_3 must be in N. Consider the following cases.

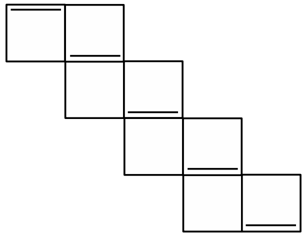

Figure 7: Polyomino chain S_k (k even) with maximal matching M.

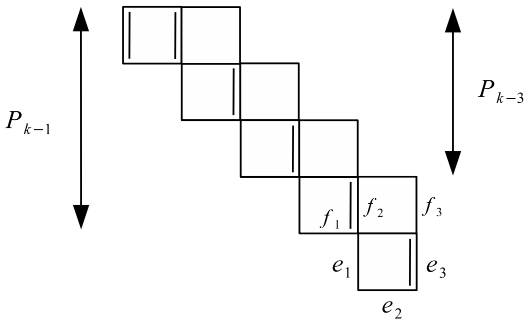

Figure 8: Polyomino chain S_k (k odd) with maximal matching M.

(a) If $e_1 \in N$, then also $e_3 \in N$ or $f_3 \in N$. Therefore, for the graph S_{k-3} (see Figure 8) it must hold $s(S_{k-3}) \leq \frac{k-3}{2}$, which is a contradiction with Case 1.

(b) If $e_2 \in N$, then for the graph S_{k-1} (see Figure 8) it must hold $s(S_{k-1}) \leq \frac{k-1}{2}$, which is a contradiction with Case 1.

(c) If $e_3 \in N$, then also one of the edges e_1, f_1, f_2 must be in N. If $e_1 \in N$ or $f_1 \in N$, then for the graph S_{k-3} (see Figure 8) it must hold $s(S_{k-3}) \leq \frac{k-3}{2}$, which is a contradiction with Case 1. Therefore, suppose that $f_2 \in N$. But in this case we can use similar reasoning and either obtain a contradiction with the Case 1 or eventually obtain a matching M', which is a contradiction since $|M'| > |N|$.

Since we obtain a contradiction in every case, it follows that every maximal matching of S_k has at least $\frac{k+1}{2}+1$ edges. Since $\frac{k+1}{2}+1 = \lceil \frac{k}{2} \rceil + 1$ it follows $s(S_k) \geq \lceil \frac{k}{2} \rceil + 1$ and we are done. $\square$

4 Hexagonal animals

In this section we prove some results regarding the saturation number of benzenoid chains and coronenes.

4.1 Benzenoid chains

A benzenoid chain of length h will be denoted by B_h. If all interior hexagons of a benzenoid chain are straight, the chain is called a *polyacene* and denoted by A_h.

Saturation number of benzenoid chains has been already studied in a recent paper coauthored by one of the present authors [5]. We quote without proof some basic results established there.

Proposition 4.1 ([5]). *Let B_h be a benzenoid chain with h hexagons. Then $s(B_h) \geq h+1$.*

Proposition 4.2 ([5]). *For any h it holds*

$$s(B_h) + 1 \leq s(B_{h+1}) \leq s(B_h) + 2.$$

Proposition 4.3 ([5]). *$s(B_h) = h + 1$ if and only if $B_h = A_h$.*

Let $B_{h,1}$ denote a chain of length $h = k+m$ in which hexagon h_k is kinky and all other hexagons are straight. An example is shown in Figure 9. Furthermore, let $B_{h,k}$ denote a benzenoid chain of length h with exactly k kinky hexagons.

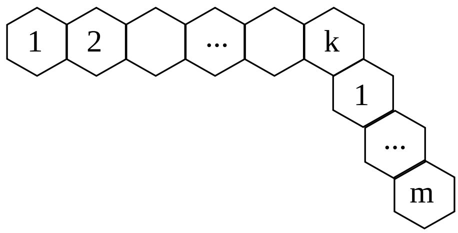

Figure 9: A chain with one kinky hexagon.

Proposition 4.4 ([5]). *For any h it holds*

$$s(B_{h,1}) = h + 2.$$

Hence one kinky hexagon means one more edge in the smallest maximal matching.

The following claim was stated in [5] as Proposition 5.

Proposition 4.5 ([5]). *Let $B_{h,k}$ be a benzenoid chain of length h with k kinky hexagons such that no two kinky hexagons are adjacent. Then $s(B_{h,k}) = h + k + 1$.*

However, we show in Proposition 4.7, Proposition 4.8, and Proposition 4.9 that the above proposition provides only an upper bound for the saturation number, which is evident from the following proposition.

Proposition 4.6. *Let $B_{h,k}$ be a benzenoid chain of length h with k kinky hexagons. Then $s(B_{h,k}) \leq h + k + 1$.*

Proof. Let M be a matching of $B_{h,k}$ obtained by taking all edges shared by two hexagons, one additional edge in each terminal hexagon and all edges connecting vertices of degree two in kinky hexagons. See Figure 10 for an example.

It is easy to see that M is a maximal matching and $|M| = h + k + 1$. Therefore, we are done. □

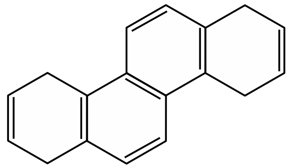

Figure 10: Maximal matching M.

However, in the same graph shown in Figure 10 we can construct a smaller maximal matching by simply taking all vertical edges. Hence $h + k + 1$ is only an upper bound on $s(B_{h,k})$ and it can be improved in particular cases.

Let B_h be a chain of length h. A *straight segment* in B_h is any sequence of consecutive straight hexagons. Equivalently, it is any sub-word made of consecutive L's in the LA sequence of B_h. The number of consecutive straight hexagons is the *length* of the straight segment.

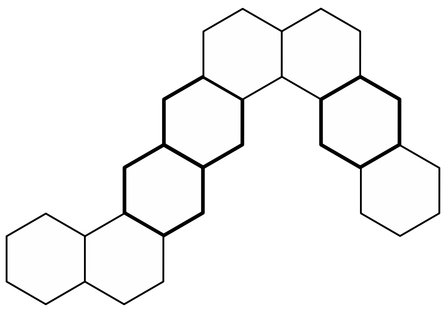

Figure 11: A benzenoid chain B_8 with two straight segments (labelled with bold edges), one of length 2 and one of length 1.

In the following we consider the saturation number of benzenoid chains where all straight segments are of length one and no two kinky hexagons are adjacent. It turns out we have to distinguish between three cases. In all of them the upper bound from Proposition 4.6 is improved.

Proposition 4.7. *Let $B_{2k+1,k}$ be a benzenoid chain such that all straight segments are of length one and no two kinky hexagons are adjacent. Then*

$$s(B_{2k+1,k}) \leq \frac{1}{4}\big(10k + 9 - (-1)^k\big).$$

Proof. We build $B_{2k+1,k}$ from left to right by adding blocks of 4 consecutive hexagons at a time. Each block has the form $LALL$ and it is added on the rightmost hexagon of the already constructed chain so that it becomes a kinky hexagon in the new chain. To show an upper bound for the saturation number, we construct a maximal matching M of $B_{2k+1,k}$. For the first four hexagons we need six edges in a maximal matching such that the edge connecting the first and the second block of hexagons is in the matching. See Figure 12.

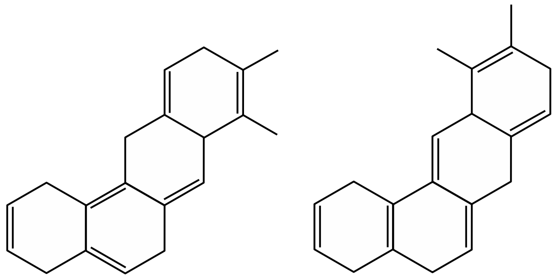

Figure 12: Two possibilities for a maximal matching M of the first block.

Afterwards, we can always add four hexagons at a price of five new edges in a maximal matching. Let l be the number of blocks in $B_{2k+1,k}$. We consider two cases.

- If k is odd, then $4 \mid (2k-2)$ and $l = \frac{2k-2}{4} = \frac{k-1}{2}$ and we have three additional hexagons in a benzenoid chain. For these three hexagons, we need 4 additional edges in a maximal matching. We obtain $|M| = 6 + 5(l-1) + 4 = 10 + 5 \cdot \frac{k-3}{2} = \frac{5k+5}{2}$.
- If k is even, then $l = \frac{2k}{4} = \frac{k}{2}$ and we have one additional hexagon in a benzenoid chain. For this hexagon, we need 1 additional edge in a maximal matching. Therefore, we get $|M| = 6 + 5(l-1) + 1 = 7 + 5 \cdot \frac{k-2}{2} = \frac{5k+4}{2}$.

Combining both cases, we obtain $|M| = \frac{1}{4}\big(10k + 9 - (-1)^k\big)$. □

Proposition 4.8. *Let $B_{2k+2,k}$, $k \in \mathbb{N}$, be a benzenoid chain such that all straight segments are of length one and no two kinky hexagons are adjacent. Then*

$$s(B_{2k+2,k}) \leq \frac{1}{4}\big(10k + 13 - (-1)^k\big).$$

Proof. We build $B_{2k+2,k}$ from left to right by adding blocks of 4 consecutive hexagons at a time. Each block has the form $LALL$ or each block has the form $LLAL$ (before adding) and it is added on the rightmost hexagon of the already constructed chain. Because of the symmetry, we can assume that each block has the form $LALL$ (otherwise we can start from right to left). The new block is added on the last hexagon such that it becomes a kinky hexagon. To show an upper bound for the saturation number, we construct a maximal matching M of $B_{2k+2,k}$. For the first four hexagons we need six edges in a maximal matching such that the edge connecting the first and the second block of hexagons is in the matching. Afterwards, we can always add four hexagons at a price of five new edges in a maximal matching. Let l be the number of blocks in $B_{2k+2,k}$. We consider two cases.

- If k is odd, then $4 \mid (2k+2)$ and $l = \frac{2k+2}{4} = \frac{k+1}{2}$. We obtain $|M| = 6 + 5(l-1) = 6 + 5 \cdot \frac{k-1}{2} = \frac{5k+7}{2}$.
- If k is even, then $l = \frac{(2k+2)-2}{4} = \frac{k}{2}$ and we have two additional hexagons in a benzenoid chain. For these two hexagons, we need 2 additional edges in a maximal matching. Therefore, we get $|M| = 6 + 5(l-1) + 2 = 8 + 5 \cdot \frac{k-2}{2} = \frac{5k+6}{2}$.

Combining both cases, we obtain $|M| = \frac{1}{4}\big(10k + 13 - (-1)^k\big)$. □

Proposition 4.9. *Let $B_{2k+3,k}$, $k \in \mathbb{N}$, be a benzenoid chain such that all straight segments are of length one and no two kinky hexagons are adjacent. Then*

$$s(B_{2k+3,k}) \le \frac{1}{4}\big(10k + 19 + (-1)^k\big).$$

Proof. We build $B_{2k+3,k}$ from left to right by adding blocks of 4 consecutive hexagons at a time. Each block has the form $LLAL$ (before adding) and it is added on the right-most hexagon of the already constructed chain. The new block is added such that the first hexagon of this block becomes a kinky hexagon. To show an upper bound for the saturation number, we construct a maximal matching M of $B_{2k+3,k}$. For the first four hexagons we need six edges in a maximal matching such that the edge connecting the first and the second block of hexagons is in the matching. Afterwards, we can always add four hexagons at a price of five new edges in a maximal matching (such that the edge connecting that block with the next block is in the matching). Let l be the number of blocks in $B_{2k+3,k}$. We consider two cases.

- If k is odd, then $4 \mid ((2k+3)-1)$ and we have to add one additional hexagon (for this hexagon we need one additional edge). Hence, $l = \frac{2k+2}{4} = \frac{k+1}{2}$. We obtain $|M| = 6 + 5(l-1) + 1 = 7 + 5 \cdot \frac{k-1}{2} = \frac{5k+9}{2}$.
- If k is even, then $4 \mid ((2k+3)-3)$ and we have to add three additional hexagons (for this three hexagons we need four additional edges in a maximal matching). Hence, $l = \frac{2k}{4} = \frac{k}{2}$. Therefore, we get $|M| = 6 + 5(l-1) + 4 = 10 + 5 \cdot \frac{k-2}{2} = \frac{5k+10}{2}$.

Combining both cases, we obtain $|M| = \frac{1}{4}\big(10k + 19 + (-1)^k\big)$. □

4.2 Coronenes

In this section we prove bounds for the saturation number of coronenes. These highly symmetric benzenoid systems have long been attracting the attention of both theoretical and experimental chemists. They are suggested as markers for vehicle emissions, since they are produced by incomplete combustion of organic matter. Coronene H_1 is just a single hexagon, and H_k is obtained from H_{k-1} by adding a ring of hexagons around it. See Figure 13 for an example of coronene H_4.

Proposition 4.10. *Let H_k be a coronene. Then*

$$\frac{3}{2}k^2 \le s(H_k) \le \begin{cases} 2k^2, & 3 \mid (k-1) \\ 2k^2 + \frac{4k}{3}, & 3 \mid k \\ 2k^2 + \frac{2k+2}{3}, & 3 \mid (k-2). \end{cases}$$

Proof. Obviously, every coronene has a perfect matching. Since the number of vertices in H_k is $6k^2$, it follows by Lemma 2.1 that $s(H_k) \ge \frac{3}{2}k^2$.

For the upper bound, we will consider just the case when $3 \mid (k-1)$, since the proofs for other two cases are almost the same. To prove this case, we construct a maximal matching M for H_k. In the matching we put all the vertical edges lying in the center layer of the coronene H_k. Since there are $2k-1$ hexagons in the center layer, we obtain $2k$ edges in the matching M. See Figure 13. Next, we continue at the top half of the coronene with alternating non-vertical and vertical edges such that two layers of edges are needed

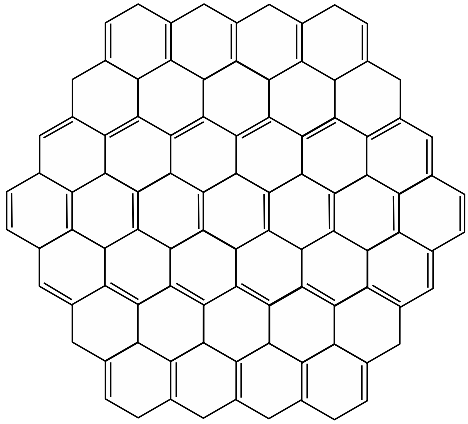

Figure 13: A coronene H_4.

for every three layers of hexagons. Furthermore, for every non-vertical layer of edges we need one additional vertical edge. Let x be the number of edges in M in the top half of the coronene. Then

$$\begin{aligned} x &= (2k-1)+(2k-3)+(2k-4)+(2k-6)+\cdots+(k+3)+(k+1) = \\ &= \frac{2(k-1)}{3}\cdot(2k) - \big(1+3+4+6+\cdots+(k-3)+(k-1)\big) = \\ &= \frac{4k^2-4k}{3} - \left(\frac{k^2-k}{2} - \big(2+5+\cdots+(k-2)\big)\right) = \\ &= \frac{4k^2-4k}{3} - \left(\frac{k^2-k}{2} - \frac{k^2-k}{6}\right) = \\ &= k^2-k. \end{aligned}$$

Finally, we obtain $|M| = 2k+2x = 2k+2(k^2-k) = 2k^2$. □

In the next proposition we improve the lower bound for any $k \geq 7$.

Proposition 4.11. *Let H_k be a coronene where $k > 1$. Then*

$$s(H_k) \geq 2k^2 - 3k - 1.$$

Proof. For any H_k, $k \geq 2$, one can construct a disk-shaped fullerene by taking another copy of H_k and connecting the borders in the following way. We insert $6k$ edges between vertices of degree 2 such that end-vertices lie in different copies of H_k. Obviously, this can be done in such a way that the resulting graph F is planar with only pentagonal and hexagonal faces. Since F is also 3-regular, it is a fullerene with $12k^2$ vertices.

Let M' be a maximal matching in each copy of H_k. Then this matching can be extended to a maximal matching M of a graph F by adding at most $6k$ edges between two copies of H_k. Therefore, $|M| \leq 2|M'|+6k$. From Theorem 4.1 in [2] it follows $|M| \geq \frac{|V(F)|}{3} - 2 = 4k^2-2$. Therefore, we obtain $2|M'|+6k \geq 4k^2-2$. Finally, $|M'| \geq 2k^2-3k-1$. □

Concluding remarks

In the paper we have established some bounds and also exact values for the saturation number of certain families of lattice animals. However, there are still many open problems regarding the exact values for the saturation number of different families of graphs.

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