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THE ANTI-KEKULÉ NUMBER OF THE INFINITE TRIANGULAR, RECTANGULAR AND HEXAGONAL GRIDS

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Abstract. The anti-Kekulé number is the smallest number of edges that must be removed from a connected graph with a perfect matching so that the graph remains connected, but has no perfect matching. In this paper the values of the Anti-Kekulé numbers of the infinite triangular, rectangular and hexagonal grids are found, and they are, respectively, 9, 6 and 4.

1. Introduction

Graph theory models have extensively been used as predictors of properties of chemical compounds (see [6, 7] and references within). A perfect matching [4] in a graph corresponds to the notion of a Kekulé structure in chemistry, and plays a very important role in the analysis of benzenoid systems, fullerenes and other carbon cages [2, 5]. For example, it is well-known that carbon compounds without Kekulé structures are unstable [5].

The anti-Kekulé number was introduced in [10] and further studied in [3, 9]. This paper continues these studies. It is well-known that the plane can be regularly tiled only by triangles, squares and hexagons. These three types of tilings result in three (infinite) grids: the triangular grid, the rectangular grid, and the hexagonal grid. In this paper, we show that the anti-Kekulé number of the triangular grid is 9, of the rectangular grid is 6 and of the hexagonal grid is 4.

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2. Basic definitions and preliminaries

Throughout this paper, we use standard graph-theoretical terms and notation [1, 8, 11]. Let G be a connected graph with at least one perfect matching (Kekulé structure). Let $E(G)$ denote the set of edges of G and $V(G)$ its set of vertices. Let $S \subseteq E(G)$. Denote by $G - S$ the graph obtained by deleting the edges in S from G. Edges in S will be called deleted edges. If $G - S$ is connected and has no perfect matching, then we say that S is anti-Kekulé set. The cardinality of the smallest anti-Kekulé set is called the anti-Kekulé number of graph G and it is denoted by $akn(G)$.

Borrowing chemical terminology, given a perfect matching M, we say an edge is a double bond if it is contained in M, and otherwise, we call it a single bond.

3. Main results

As the main results, we give three theorems in which the anti-Kekulé numbers of the infinite triangular, rectangular and hexagonal grids are calculated. These infinite graphs are called G_3, G_4 and G_6, respectively.

Theorem 3.1. *The anti-Kekulé number of the hexagonal grid, G_6, is equal to 4.*

Proof. From Figure 1, it can be easily seen that $akn(G_6) \leq 4$. Just note that the two back vertices can not both be met by any perfect matching.

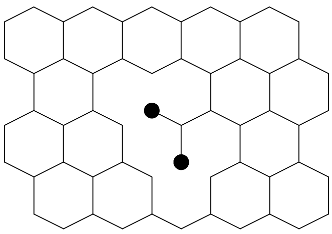


Figure 1. Anti-Kekulé set consisting of four edges

Now, let us prove that $akn(G_6) \geq 4$. Suppose to the contrary that there is a set D consisting of at most three edges such that $G_6 - D$ is connected, but has no perfect matching. Of course, we may assume that $|D| = 3$.

We say that a hexagon is conjugated by a perfect matching M if it contains three double bonds (that is, three edges of M). Note that each hexagon can be conjugated in two different ways as in Figure 2. Divide the hexagons of the hexagonal grid into three classes as in Figure 3.

One can easily see that there is a set CA (resp. CB, CC) of perfect matchings that consist solely of double bond edges of hexagons of A (resp. B, C).

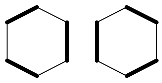


FIGURE 2. Two ways a hexagon can be conjugated

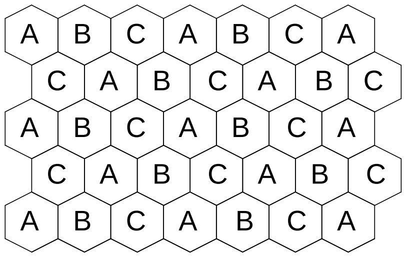


FIGURE 3. Division of hexagons in three classes

It follows that there is a hexagon denoted by H_A in A (resp. H_B in B, H_C in C) that contains at least two edges of D. Since $|D| = 3$, the three hexagons H_A, H_B and H_C each contain exactly 2 edges in D. Since no two hexagons share two edges, it follows that one edge of D is shared by H_A and H_B; one by H_A and H_C; and one by H_B and H_C. This is possible only when all three edges are incident to the same vertex, but then $G_6 - D$ is disconnected, a contradiction. Hence, $|D| \geq 4$. □

THEOREM 3.2. *The anti-Kekulé number of the infinite rectangular grid, G_4, is equal to 6.*

PROOF. From Figure 2 we see that $akn\,(G_4) \leq 6$. Just note that the two black vertices can not both be met by any perfect matching. Let us prove that

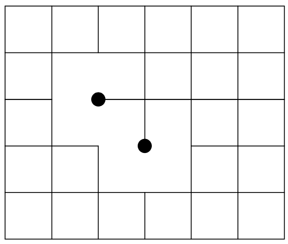


FIGURE 4. An anti-Kekulé set consisting of 6 edges

$akn\,(G_4) \geq 6$. Suppose to the contrary that there is a set D consisting of at most five edges such that $G_6 - D$ is connected, but has no perfect matching. Of course, we may assume that $|D| = 5$. We say that a line is conjugated by M

if all its vertices are met by edges of M that lay on that line. Of course, each line can be conjugated in two ways as shown in Figure 5. Since, $G_4 - D$ has

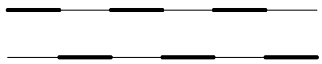


FIGURE 5. Two ways in which a line can be conjugated

no perfect matching, it follows that there are at least one horizontal and one vertical line each containing two edges of D. Since $|D| = 5$, there is exactly one vertical line vl and one horizontal line hl containing at least two edges of D each. Let vertex v be the intersection of these two lines. Distinguish between the following five cases:

CASE 1: There are four deleted edges incident to v.

In this case, the graph is disconnected which is a contradiction.

CASE 2: There are three deleted edges incident to v.

Without loss of generality, we may assume that we have the following situation:

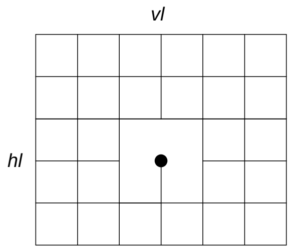


FIGURE 6. Graph for Case 2.

Denote by D' the set of remaining two edges in D. Denote by B_1 the set of bold lines on the left hand-side of Figure 7 and by B_2 the set of bold lines on the right hand-side in Figure 7.

Note that D' has at least one edge on vl. Hence, $(B_1 \cup B_2) \cap D$ contains at most one element. Since $B_1 \cap B_2$ has only one edge and it is not in D, it follows that at least one of sets $B_1 \cap D'$ and $B_2 \cap D'$ is empty. Without loss of generality, let us assume that $B_1 \cap D'$ is empty. Note that each line represented by a dotted line contains at most one edge in D. Hence, it can be conjugated (choosing conjugation that avoids that edge). But, then there is a Kekulé structure in $G_4 - D$ that consists of the edges in B_1 and in conjugated dotted lines. This is a contradiction.

CASE 3: There are two deleted edges incident to v and they lie on the same line.

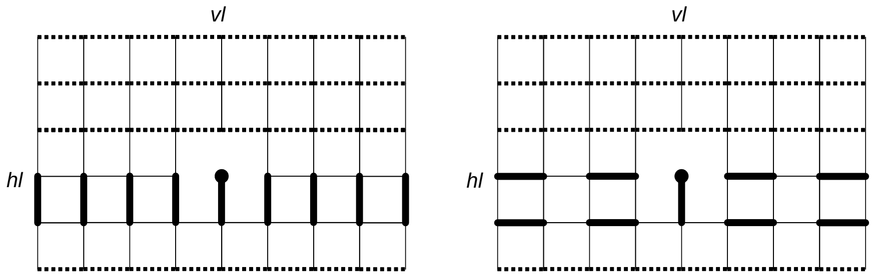


Figure 7. Sets B_1 and B_2 and conjugated lines

Without loss of generality, we may assume that we have the following situation:

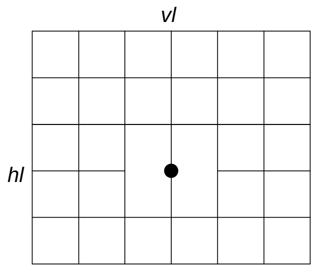


Figure 8. Graph for Case 3

The proof goes analogously to that of Case 2 by observing the following figure:

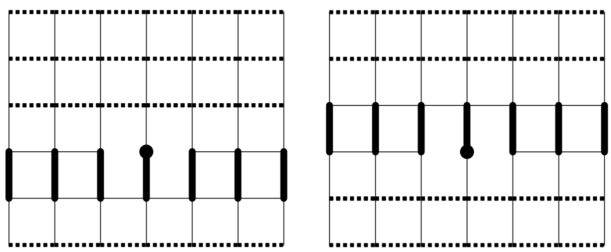


Figure 9. Case 3: Disjoint sets of double bonds and sets of conjugated lines.

Case 4: There are two deleted edges incident to v and they are on different lines.

Without loss of generality, we may assume that we have the following situation:

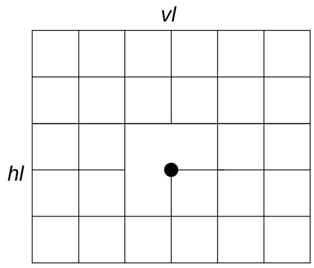


FIGURE 10. Graph for Case 4.

The proof goes analogously to that of Case 2 by observing the following figure:

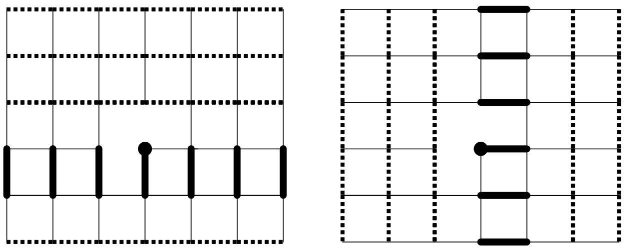


FIGURE 11. Case 4: Disjoint sets of double bonds and sets of conjugated lines.

CASE 5: There is at most one deleted edge incident to v.

Without loss of generality, we may assume that we have the following situation:

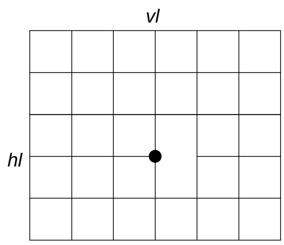
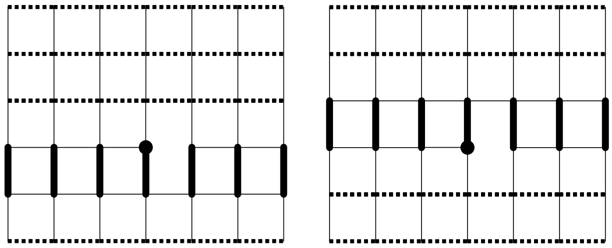


FIGURE 12. Graph for Case 5.

The proof goes analogously to that of Case 2 by observing the following figure:



Case 5: Disjoint sets of double bonds and sets of conjugated lines.

All the cases are exhausted and the theorem is proved. ∎

Before the following theorem, we need some auxiliary results. Suppose that a coordinate system is introduced in G_4.

LEMMA 3.3. *Let $P \subseteq E(G_4)$ be a finite set of edges. Let C be the component of the graph $G_4 - P$. Then,*

$$\begin{aligned} |P| \quad \geq \quad & 2 \cdot (\max \{x(T) : T \in V(C)\} - \min \{x(T) : T \in V(C)\} + 1) + \\ & 2 \cdot (\max \{y(T) : T \in V(C)\} - \min \{y(T) : T \in V(C)\} + 1). \end{aligned}$$

PROOF. Just note that above and below (not necessarily immediately above and below) each point in C, there is at least one edge in P; and also to the left and to the right (not necessarily immediately to the left and to the right) of each point in C, there is at least one edge in P. ∎

From here, it directly follows that:

LEMMA 3.4. *If C is a component of $G_4 - P$ and $|P| \leq 5$, then C consists of a single vertex and P contains all edges incident to that vertex.*

LEMMA 3.5. *Let C be a connected component of $G_4 - P$ and $|P| = 6$. Then either:*
1) C consists of a single vertex and P contains all edges incident to that vertex, or
2) C consists of two vertices and P contains all edges incident to these vertices (except one connecting these two vertices).

Now, we can prove:

THEOREM 3.6. *The anti-Kekulé number of the infinite triangular grid, G_3, is equal to 9.*

REMARK 3.7. For the sake of simplicity, we draw the triangular grid in the following (isomorphic) form:

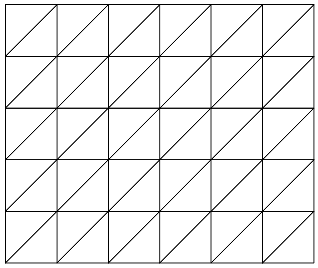


FIGURE 13. Triangular grid

PROOF. From Figure 14, it can be easily seen that $akn(G_3) \leq 9$. Just note that the two black vertices can not both be met by any perfect matching.

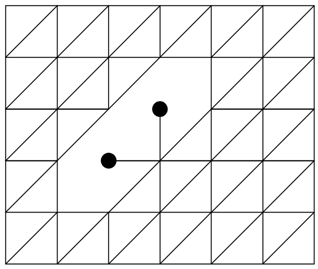


FIGURE 14. An anti-Kekulé set consisting of nine edges.

Let us prove that $akn(G_3) \geq 9$. Suppose to the contrary that there is a set D consisting of at most eight edges such that $G_3 - D$ is connected, but has no perfect matching. The edges of G_3 can be divided into three groups according to their direction: the set of horizontal ones, vertical ones and skew ones. Denote by D_h, D_v and D_s the sets of horizontal, vertical and skew edges in D, respectively. Denote by $G_{h,v}$ the subgraph of G_3 consisting of only horizontal and vertical edges, and define $G_{h,s}$ and $G_{v,s}$ analogously. Note that $G_{h,v}$, $G_{h,s}$ and $G_{v,s}$ are all isomorphic to G_4.

Without loss of generality, we may assume that $|D_h| \leq |D_v| \leq |D_s|$. Note that $|D_h| \geq 2$, because otherwise there is a perfect matching in $G_3 - D$ consisting of conjugated horizontal lines. From $|D_h| + |D_v| + |D_s| \leq 8$, it follows that $|D_h| = 2$.

Note that $|D_h| + |D_v| \leq 5$. From Theorem 2, it follows that $D_h \cup D_v$ is not an anti-Kekulé set in $G_{h,v}$. Since, $G_{h,v} - (D_h \cup D_v)$ has no perfect matching, it follows that it is disconnected. From Lemma 4, it follows that there is a vertex w such that all horizontal and vertical edges incident to w are in D. Distinguish two cases:

CASE 1: $|D_h| + |D_s| \leq 5$.

Analogously as above, it follows that $D_h \cup D_s$ is not an anti-Kekulé set in $G_{h,s}$ and hence $G_{h,s} - (D_h \cup D_s)$ is disconnected. From Lemma 4, it follows that there is a vertex w' such that all horizontal and skew edges incident to w' are in D. Since there are only two horizontal edges in D, it follows that $w' = w$. But then, all edges incident to w are in D, and $G_3 - D$ is disconnected, which is a contradiction.

CASE 2: $|D_h| + |D_s| \geq 6$.

In this case $|D_h| = |D_v| = 2$ and $|D_s| = 4$. Since, both horizontal and both vertical edges in D are incident to w, it follows that at least one of the skew edges incident to w is not in D. But then, the following figure gives a perfect matching in G_3 which is a contradiction. This proves the theorem.

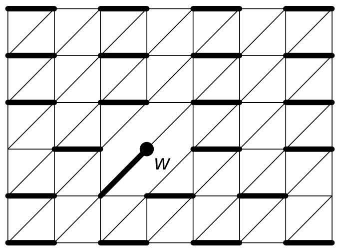


FIGURE 15. Perfect matching in $G_3 - D$

□

As an open problem, we propose the analysis of the anti-Kekulé number of multidimensional grids.

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