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GRAPHS WHERE EACH SPANNING TREE HAS A PERFECT MATCHING

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Abstract. An edge subset S of a connected graph G is called an anti-Kekulé set if $G-S$ is connected and has no perfect matching. We can see that a connected graph G has no anti-Kekulé set if and only if each spanning tree of G has a perfect matching. In this note, we characterize all graphs where each spanning tree has a perfect matching. In addition, we show that if G is a connected graph of order $2n$ for a positive integer $n \geq 4$ and size m whose each spanning tree has a perfect matching, then $m \leq \frac{(n+1)n}{2}$, with equality if and only if $G \cong K_n \circ K_1$.

1. Introduction

All graphs considered in this paper are finite and simple. We refer to [3] for undefined notation and terminology. For a graph $G = (V(G), E(G))$, we denote the *order* and the *size* of G, respectively, by $v(G)$ and $e(G)$. For a vertex $v \in V(G)$, the *degree* of v, denoted by $d_G(v)$, is the number of edges incident with v in G; the *neighborhood* of v, denoted by $N_G(v)$, is the set of vertices adjacent to v in G. As usual, the complete graph, the path, and the cycle of order $n \geq 1$ are denoted by K_n, P_n, and C_n, respectively. A *matching* in a graph G is a set of pairwise nonadjacent edges. If M is a matching, the two ends of each edge of M are said to be *matched* under M, and each vertex incident with an edge of M is said to be *covered* by M. A *perfect matching* (or *Kekulé structure* in chemistry) of a graph G is a matching which covers every vertex of G. An edge of G is a *fixed double (single)* edge if it belongs to all (none) of the perfect matchings of G. Both fixed double edges and fixed single edges are called *fixed* edges. A bipartite graph with a perfect matching is called *normal (or elementary)* if it is connected and has no fixed edges.

Let G be a connected graph. An edge subset S of G is called an *anti-Kekulé set* of G if $G-S$ is connected and has no perfect matching. The cardinality of a minimum anti-Kekulé set of G is called the anti-Kekulé

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number and is denoted by $ak(G)$. The notion of anti-Kekulé sets and anti-Kekulé number were first introduced by Vukičević and Trinajstić [10] in 2007.

Vukičević and Trinajstić [10, 11] showed that the anti-Kekulé number of benzenoid parallelograms is 2 and the anti-Kekulé number of cata-condensed hexagonal systems equals either 2 or 3. Cai and Zhang [4] showed that for a hexagonal system H with more than one hexagon, $ak(H) = 0$ if and only if H has no perfect matching, $ak(H) = 1$ if and only if H has a fixed double edge, and $ak(H)$ is either 2 or 3 for the other cases. Further, by applying perfect path systems, they gave a characterization whether $ak(H) = 2$ or 3, and presented an $O(n^2)$ algorithm for finding a smallest anti-Kekulé set in a normal hexagonal system, where n is the number of its vertices.

Vukičević [9] showed that the anti-Kekulé number of the icosahedron fullerene C_{60} (buckminsterfullerene) is 4. Kutnar et al. [5] proved that the anti-Kekulé number of all fullerenes is either 3 or 4 and that for each leapfrog fullerene the anti-Kekulé number can be established by observing a finite number of cases not depending on the size of the fullerene. Yang, Ye, Zhang, Lin [12] showed that the anti-Kekulé number is always equal to 4 for all (5,6)-fullerenes. Recently, Zhao and Zhang [15] gave a complete classification of (4,5,6)-fullerences in terms of the anti-Kekulé number is 3 or 4.

Veljan and Vukičević [8] found that the values of the anti-Kekulé numbers of the infinite triangular, rectangular, and hexagonal grids are, respectively, 9, 6, and 4. Among other things, it was shown that the anti-Kekulé number of cata-condensed phenylenes is 3 in [14]. Ye [13] showed that, if G is a cyclically $(r+1)$-edge-connected r-regular graph ($r \geq 3$) of even order, then either the anti-Kekulé number of G is at least $r + 1$, or G is not bipartite, and the smallest odd cycle transversal of G has at most r edges. Lü et al. [6] showed that computing the anti-kekulé number of bipartite graphs is NP-complete.

In spite of the above known results on anti-Kekulé number of a graph, a fundamental problem has not been solved yet: what kinds of graphs do not have an anti-Kekulé set? Indeed, there exist some connected graphs, for instance, K_2 and all even cycles, which do not have an anti-Kekulé set. For such a graph G, $ak(G)$ is not defined. The aim of this note is to characterize all these graphs. Our approach is to construct all such graphs from K_2 and all even cycles by certain operations.

To this end, let us define recursively a family $\mathcal{G}$ of graphs.

(1) K_2 and all even cycles belong to $\mathcal{G}$;

(2) Assume that H is a connected graph of order $p \geq 2$ with vertex set $\{u_1, \ldots, u_p\}$ and $F_i \in \mathcal{G}$ for each $i \in \{1, \ldots, p\}$, where $H, F_1, \ldots, F_p$ are pairwise vertex-disjoint. For each i, take a vertex $v_i \in V(F_i)$. The graph obtained from $H, F_1, \ldots, F_p$ by identifying the vertices u_i and v_i for each i, denoted by $H[F_1(u_1v_1), \ldots, F_p(u_pv_p)]$ (or simply by $H[F_1, \ldots, F_p]$), belongs to $\mathcal{G}$, as shown in Figure 1.

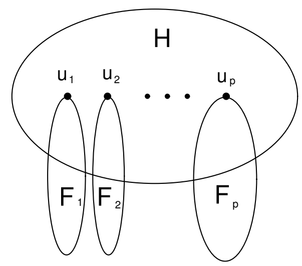
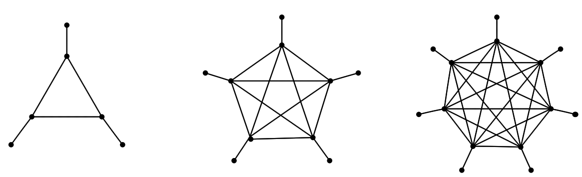


FIGURE 1. $H[F_1, \dots, F_p]$

Note that every tree with a perfect matching belong to $\mathcal{G}$. For instance, $P_4 \cong K_2[K_2, K_2]$, in our notation. It is well-known (see [2, p. 80]) that a tree has a perfect matching if and only if $c_o(T - v) = 1$ for all vertex $v \in V(T)$. Indeed, it is not hard to show that the family $\mathcal{T}$ of trees with a perfect matching can be recursively constructed in the following way:

(1) $K_2 \in \mathcal{T}$,

(2) if $T_i \in \mathcal{T}$ for $1 \leq i \leq 2$ with $V(T_1) \cap V(T_2) = \emptyset$, then $T \in \mathcal{T}$, where T is obtained from T_1 and T_2 by joining a vertex of T_1 to that of T_2 with an edge.



$K_3 \circ K_1$ $K_5 \circ K_1$ $K_7 \circ K_1$

FIGURE 2. The corona $K_n \circ K_1$

The *corona* $G \circ K_1$ of a graph G is the graph obtained from G by adding an edge between each vertex of G and its copy. Observe that $G \circ K_1 \in \mathcal{G}$ for any connected graph G, since $G \circ K_1 \cong G[K_2, K_2, \cdots, K_2]$ under our notation above. The coronas $K_n \circ K_1$ are given for some values of n, as shown in Figure 2. The join of two vertex-disjoint graphs G and H, denoted by $G \vee H$, is the graph obtained from $G \cup H$ by joining each vertex of G to all vertices of H.

We present our main theorem as follows.

Theorem 1.1. *Let G be a connected graph. The following statements are equivalent:*
(1) G has no anti-Kekulé set,
(2) Each connected spanning subgraph of G has a perfect matching,
(3) Each spanning tree of G has a perfect matching,and
(4) $G \in \mathcal{G}$.

2. Preliminary

We start with Tutte's 1-factor theorem.

Theorem 2.1 (Tutte [7]). *A graph G has a perfect matching if and only if $c_o(G-S) \le |S|$ for any $S \subseteq V(G)$, where $c_o(G-S)$ is the number of odd components of $G-S$.*

For an integer $k \ge 1$, a k-connected graph G is called *minimally k-connected* if $G-e$ is not k-connected for each $e \in E(G)$. The following property for a minimally 2-connected graph can be found in [1, p. 15].

Theorem 2.2 (Bollobás [1]). *Let G be a minimally 2-connected graph that is not a cycle. Let $V_2 \subseteq V(G)$ be the set of vertices of degree two. Then $F = G - V_2$ is a forest with at least two components. A component P of $G[V_2]$ is a path and the end vertices of P are not joined to the same tree of the forest F.*

A *cut vertex* of a graph G is a vertex v such that $c(G-v) > c(G)$, where $c(G)$ denotes the number of components of G. A *decomposition* of a graph G is a family $\mathcal{F}$ of edge-disjoint subgraphs of G such that $\cup_{F\in\mathcal{F}} E(F) = E(G)$. A *separation* of a connected graph is a decomposition of the graph into two nonempty connected subgraphs of orders at least two which have just one vertex in common. This common vertex is called a *separating vertex* of the graph. A cut vertex is clearly a separating vertex. If the graph under consideration is connected, the two concepts, separating vertex and cut vertex, are identical. A graph is nonseparable if it is connected and has no cut vertices; otherwise, it is separable. Thus, a nonseparable graph other than K_2 is 2-connected. A *block* of a graph G is a subgraph that is nonseparable and is maximal with respect to this property. Further, a block of G is called an *end block* if it contains just one cut vertex of G.

To show our main theorem, we need the following two lemmas.

Lemma 2.3. *If G is a nonseparable graph whose each spanning tree has a perfect matching, then it is isomorphic to K_2 or an even cycle.*

Proof. By the assumption, G has even order n. Suppose to the contrary that G is isomorphic to neither K_2 nor an even cycle. Then $n \ge 4$ and G is 2-connected. We consider the following two cases.

Case 1: G contains a Hamilton cycle C.

Label the vertices of C as $v_1, v_2, \ldots, v_n$ in the cyclic order. Since $G \ncong C_n$, there is a chord for C. Without loss of generality, let v_1v_k be such an edge. Since $3 \le k \le n-1$, $T = C - v_{k-2}v_{k-1} - v_{k+1}v_{k+2} + v_1v_k$ is a spanning tree of G without a perfect matching, a contradiction.

Case 2: G contains no Hamilton cycle.

Let H be a minimally 2-connected spanning subgraph of G. Then H is not a cycle. Let V_2 be the set of vertices with degree 2 in H. By Theorem 2.2, $H - V_2$ is a forest F with at least two components. Take a vertex $v \in V(F)$ with $0 \le d_F(v) \le 1$. Since $d_H(v) \ge 3$, v has two neighbors, say u and w, in V_2. Again by Theorem 2.2, each of u and w is an endvertex of a path component in $H[V_2]$, and such a path joins distinct components of the forest F. We have that $H-u-w$ is connected. Otherwise $H-v$ is disconnected, contradicting that H is 2-connected. Let T_{uw} be a spanning tree of $H-u-w$, and let T be the tree obtained from T_{uw} adding the vertices u, w and the edges vu and vw. However, T is a spanning tree of G without a perfect matching, a contradiction. $\square$

Lemma 2.4. *For $G \in \mathcal{G}$ and $F \in \mathcal{G}$ with $uv \in E(G)$ and $d_G(v) = 1$, let G' be the graph obtained from $G - v$ and F by identifying a vertex w of F to u. Then $G' \in \mathcal{G}$.*

Proof. We proceed by induction on the order n of G. If $n = 2$, then $G' \cong F$ and the result is trivial. Now let $n \geq 4$. Then G is neither K_2 nor an even cycle. By the definition of graph class $\mathcal{G}$, there exists a connected graph H of order $p \geq 2$ with vertex set $\{u_1, \ldots, u_p\}$ and $F_i \in \mathcal{G}$ for each $i \in \{1, \ldots, p\}$, where $H, F_1, \ldots, F_p$ are pairwise vertex-disjoint such that $G = H[F_1, \ldots, F_p]$. Without loss of generality, let $v \in V(F_1)$. If $F_1 = K_2$, we are done, because $G' = H[F, F_2, \ldots, F_p]$. So assume that $F_1 \ncong K_2$. Let F_1' be the graph obtained from $F_1 - v$ and F by identifying vertex u of $F_1 - v$ and vertex w of F. Note that F_1 has less vertices than G does. By the induction hypothesis, $F_1' \in \mathcal{G}$, and thus $G' = H[F_1', F_2, \ldots, F_p] \in \mathcal{G}$. $\square$

It is natural to ask: What is the largest size of a graph of order $2n$ where each spanning tree has a perfect matching? The answer is clear for $n \leq 3$. It is easy to verify that K_2 and C_4 has the largest size for $n = 1$ and $n = 2$, respectively. If $n = 3$, there are exactly three graphs, i.e., C_6, $K_3 \circ K_1$ and $K_2[K_2, C_4]$, with the desired property. In general, we have the following.

Corollary 2.5. *If G is a connected graph of order $2n$ for a positive integer n and size m whose each spanning tree has a perfect matching, then $m \leq f(n)$, where*

$$f(n) = \begin{cases} 1, & \text{if } n = 1, \\ 4, & \text{if } n = 2, \\ \frac{(n+1)n}{2}, & \text{if } n \geq 3, \end{cases}$$

with equality if and only if

$$G \cong \begin{cases} K_2, & \text{if } n = 1, \\ C_4, & \text{if } n = 2, \\ C_6 \text{ or } K_3 \circ K_1 \text{ or} K_2[K_2, C_4], & \text{if } n = 3, \\ K_n \circ K_1, & \text{if } n \geq 4. \end{cases}$$

Proof. Assume that G is a connected graph of order $2n$ and size m whose each spanning tree has a perfect matching. We show $m \leq f(n)$ by induction on n. The result holds for $n \leq 3$ by the observation before this corollary, and the corresponding extremal graphs are those as listed in the statement of the corollary. Next, we further assume that $n \geq 4$. If G is nonseparable, then by Lemma 2.3, $m = 2n < \frac{(n+1)n}{2} = f(n)$ for any $n \geq 4$. So, we assume that G is separable in what follows. By Theorem 1.1, there exists a connected graph H of order $p \geq 2$ with vertex set $\{u_1, \ldots, u_p\}$ and $F_i \in \mathcal{G}$ for each $i \in \{1, \ldots, p\}$ such that $G = H[F_1, \ldots, F_p]$. Recall that $F_1, \ldots, F_p$ are pairwise vertex-disjoint and the order n_i of F_i is even for each $i \in \{1, \ldots, p\}$. If $F_i \cong K_2$ for each i, then $p = n$, and thus $m \leq e(K_n[K_2, \ldots, K_2]) = e(K_n \circ K_1) = \frac{n(n+1)}{2}$, with equality if and only if $H \cong K_n$, equivalently, $G \cong K_n \circ K_1$.

So, assume that $F_i \ncong K_2$ for some i, and let $n_p = \max\{n_i : i \in \{1, \ldots, p\}\}$, without loss of generality. Put $a = \frac{n_p}{2}$, and take the complete graph H' on the vertices $\{u_1, \ldots, u_p, u_{p+1}, \ldots, u_{p+a-1}\}$. Furthermore, let $G' = H'[F'_1, \ldots, F'_{p+a-1}]$, where

$$F'_i = \begin{cases} F_i, & \text{if } 1 \leq i \leq p-1, \\ K_2, & \text{if } p \leq i \leq p+a-1. \end{cases}$$

It is clear that $G' \in \mathcal{G}$, and for the size m' of G', observe that

$$\begin{aligned} m' - m &\geq a(p-1) - d_H(u_p) + \frac{(a+1)a}{2} - e(F_p) \\ &\geq (a-1)(p-1) + \frac{(a+1)a}{2} - e(F_p). \end{aligned}$$

If $a > 2$, then by the induction hypothesis, $e(F_p) \leq \frac{(a+1)a}{2}$. Combining this with $(a-1)(p-1) > 0$, we have $m' > m$. If $a = 2$, then $n_p = 4$, and thus $F_p \cong C_4$ or $F_p \cong P_4$. If $p \geq 3$, then $(a-1)(p-1) + \frac{(a+1)a}{2} - e(F_p) \geq 1$, and thus $m' \geq m+1$. If $p = 2$, then by the assumption $n \geq 4$ and $n_p = 4$ we have $n = 4$. Hence $m \leq 4+4+1 < 10 = e(K_4 \circ K_1)$.

Summing up the above, we conclude that $m \leq \frac{n(n+1)}{2}$ for any $n \geq 4$, with equality if and only if $H \cong K_n$ and $F_i \cong K_2$ for all i, i.e. $G \cong K_n \circ K_1$. □

3. Proof of Theorem 1.1

By the definition of an anti-Kekulé set we can see that G has no anti-Kekulé set if and only if for each $S \subseteq E(G)$ with $G - S$ being connected, $G - S$ has a perfect matching. Since $G - S$ is always a spanning subgraph of G, the latter can be expressed as "each connected spanning subgraph of G has a perfect matching". Hence statements (1) and (2) are equivalent. Further, the equivalence of (2) and (3) is evident.

Next we show the equivalence of statements (3) and (4). We proceed by induction on the order n of G.

We first consider (4) $\Rightarrow$ (3). If $G \cong K_2$ or G is an even cycle, then each spanning tree of G is isomorphic to P_n, and thus has a perfect matching. By the definition of $\mathcal{G}$ we assume that $G \cong H[F_1, \ldots, F_p]$, where H is a connected graph of order $p \geq 2$ and $F_i \in \mathcal{G}$, $i = 1, 2, \ldots, p$. For any spanning tree T of G, let $T_i = T \cap F_i$ for $i = 1, 2, \ldots, p$. Then T_i is a spanning tree of F_i. Since $F_i \in \mathcal{G}$, by the induction hypothesis, T_i has a perfect matching M_i. So, $M = \cup_{i=1}^{p} M_i$ is a perfect matching of T. This shows (4) $\Rightarrow$ (3).

To show (3) $\Rightarrow$ (4), we assume that each spanning tree of G has a perfect matching. If G is nonseparable, then by Lemma 2.3, G is an even cycle or K_2, and thus $G \in \mathcal{G}$. From now on the graph G will be separable. Let $\{G_1, G_2\}$ be a separation of G. Since the order of G is even and $|V(G_1) \cap V(G_2)| = 1$, the parity of $|V(G_1)|$ and $|V(G_2)|$ are distinct. Without loss of generality, let $n_2 = |V(G_2)|$ be even for any separation $\{G_1, G_2\}$ of G. We consider two cases.

Case 1: There exists a a separation $\{G_1, G_2\}$ of G with $n_2 \geq 4$.

Let v be the common vertex of G_1 and G_2, and let G_1' be the graph obtained from G_1 by joining a new vertex v_2 to v with an edge.

We assert that each spanning tree of G_2 (resp. G_1') has a perfect matching. Let T_1' be any spanning tree of G_1' and T_2 be a spanning tree of G_2. Then $(T_1' - v_2) \cup T_2$ is a spanning tree of G and thus has a perfect matching M. Since the order of T_2 is even, v is matched with a vertex in $V(T_2)$ under M. Thus $M \cap E(T_2)$ is a perfect matching of G_2 and $M \cap E(T_1' - v_2)$ is a perfect matching of $T_1' - v - v_2$. The latter implies that $(M \cap E(T_1' - v_2)) \cup \{vv_2\}$ is a perfect matching of T_1'. So the assertion holds. Since G_1' and G_2 each has fewer vertices than G, by the induction hypothesis we have that $G' \in \mathcal{G}$ and $G_2 \in \mathcal{G}$. By Lemma 2.4, it follows that $G \in \mathcal{G}$.

Case 2: $n_2 = 2$ for any separation $\{G_1, G_2\}$ of G.

In this case, we will show that $G \cong H \circ K_1$, where H is a nonseparable graph. Hence $G \in \mathcal{G}$. To this end, we have the following claim.

Claim. *For a cut vertex v of G,*

(i) *$G - v$ has exactly two components, one of which is a single vertex u;*
(ii) *for any $w \in N_G(v)$ other than u, we have $d_G(w) \geq 2$ and w is also a cut vertex of G.*

Proof. Let $\{G_1, G_2\}$ be a separation of G with $V(G_1) \cap V(G_2) = \{v\}$. Since $n_2 = 2$, $G - v$ has a single vertex as one component. Moreover, since G has a perfect matching, by Theorem 2.1 we have that exactly one component of $G - v$ is a single vertex u and all other components of $G - v$ are even. If $G - v$ has at least three components, we take an even component G' of $G - v$. Then $\{G[\{v\} \cup V(G')], G - V(G')\}$ is a separation of G such that $G - V(G')$ has an even order of at least 4, contradicting the assumption of Case 2. This shows (i).

Now we show (ii). If w is not a cut vertex of G, then G has a spanning tree T in which both u and w are leaves adjacent to v. It is clear that $c_o(T - v) \geq 2$. By Theorem 2.1, T has no perfect matching, a contradiction. This proves the claim. □

Let H be the graph obtained from G by deleting all vertices of degree one. Since G is connected, H is also connected. Note that G has cut vertices, and by Claim (i) each cut vertex v of G has exactly one neighbor u of degree one. To complete to show $G = H \circ K_1$, it remains to show that each vertex of H is a cut vertex of G. Since $V(H)$ contains some cut vertices of G, and by the definition of H, $d_G(w) \geq 2$ for any $w \in V(H)$. Since H is connected, by Claim (ii), it follows that each vertex of H is a cut vertex of G. $\square$

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