MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **77** (2017) 799-812

ISSN 0340 - 6253

On the Existence of F-Strong Trace of a Graph when F Induces a Forest

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(Received October 31, 2016)

Abstract

Recently, the notion of strong trace was introduced as a mathematical support for self-assembly of polypeptide. Graphs which admit parallel strong traces and antiparallel strong traces were then characterized. In this paper, we introduce the notion of F-strong trace, i.e. a strong trace whose corresponding antiparallel edges are exactly edges in $F \subseteq E$, which includes parallel strong trace ($F = \emptyset$) and antiparallel strong trace ($F = E$) as two extreme cases. Given a graph $G = (V, E)$ and $F \subseteq E$, in this paper we study the problem whether G admits an F-strong trace. We solve it when (V, F) is acyclic by proving that in this case G admits an F-strong trace if and only if $G \setminus F$ is even. We provide two examples to show that this condition is not always true when (V, F) contains cycles.

1 Background and notions

Throughout this paper we use $A \subseteq B$ and $A \subset B$ to denote A is a subset of B and A is a proper subset of B, respectively. All graphs considered in this paper are simple, connected and finite unless otherwise specified. Let $G = (V, E)$ be a graph with vertex set V and edge set E. For $v \in V$, we denote by $N(v)$ (resp. $E(v)$) the set of vertices adjacent to (resp. edges incident with) v, and by $d_G(v)$ ($d(v)$ for short) *the degree* of v in G, i.e. $d(v) = |N(v)| = |E(v)|$. We use $\delta(G)$ to denote *the minimum degree* of G, i.e. $\delta(G) = \min_{v \in V}\{d(v)\}$. A graph G is called to be *even* if $d(v)$ is even for each $v \in V$. For $F \subseteq E$, we denote by $G \setminus F$ the graph obtained from G by deleting all edges in F. An edge $e \in E$ is said to be a *cut edge* of G if its deletion results in a disconnected graph.

A *walk* in a graph G is a sequence $W = v_0e_1v_1 \cdots v_{l-1}e_lv_l$, whose terms are alternately vertices and edges of G (not necessarily distinct), such that v_{i-1} and v_i are the ends of e_i, $1 \leq i \leq l$. The walk W in a graph is *closed* if its initial and terminal vertices v_0 and v_l are identical. A *tour* of a graph G is a closed walk and an *Euler tour* is a tour that traverses each edge exactly once. A graph is *Eulerian* if it admits an Euler tour. A fundamental theorem of graph theory, known as Euler's theorem, states that G is Eulerian if and only if it is connected and even [1,2]. A *double trace* in G is a tour which traverses each edge of G exactly twice. Let T be a double trace in G and $e \in E$. We say that e is *parallel (resp. antiparallel)* (with respect to T) if e is traversed in the same (resp. opposite) direction along T. A double trace of G is said to be *parallel (resp. antiparallel)* if every $e \in E$ is parallel (resp. antiparallel).

We say that a double trace contains a *retracing* if it has an immediate succession of an edge e by its parallel copy as shown in Figure 1. Let T be a double trace in G and $v \in V$. We say that T contains a *repetition through* v if there exist $u, w \in N(v)$ such that the vertex sequence $u \to v \to w$ appears twice in T in any direction ($u \to v \to w$ or $w \to v \to u$) as shown in Figure 2. A double trace is said to be a *proper trace* if it does not contain any retracing. A proper trace is said to be a *stable trace* if it does not contain any repetition through any vertex.

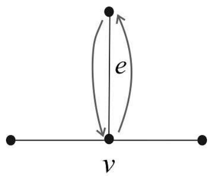


Figure 1. Retracing of an edge e.

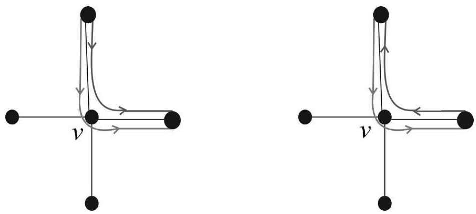


Figure 2. Repetitions through the vertex v.

In 2013, a strategy to design self-assembling polypeptide nanostructured polyhedra based on modularization using orthogonal dimerizing segments was presented in [3], and the authors succeeded in designing and experimentally demonstrating the formation of the tetrahedron, named by TET12, that self-assembles from a single polypeptide chain comprising 12 concatenated coiled coil-forming segments separated by flexible peptide hinges, see Figure 3. The notion of stable trace was introduced in [4] to provide a mathematical support for self-assembly polypeptides. But in [5], the authors found the notion deficient in dealing with graphs with either very small (≤ 2) or large (≥ 6) degree vertices, and thus they introduced the notion of the strong trace.

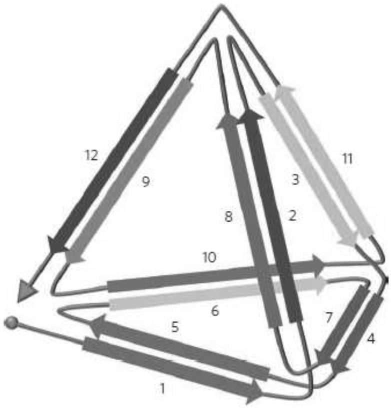


Figure 3. The tetrahedron designed from a single polypeptide chain comprising 12 concatenated coiled coil-forming segments [3].

Let T be a double trace in G of length l, $v \in V$ and $N \subseteq N(v)$. We say that T has an *N-repetition at v* if, for every $i \in \{0, \cdots, l-1\}$, if $v = v_i$ then $v_{i+1} \in N$ if and only if $v_{i-1} \in N$. An N-repetition at v is a *d-repetition* if $|N| = d$, and a d-repetition will also be called a repetition of order d. An N-repetition at v is trivial if $N = \emptyset$ or $N = N(v)$. Clearly if T has an N-repetition at v, then it also has an $N(v) \setminus N$-repetition at v. A *strong trace* is a double trace without nontrivial repetitions. Parallel and antiparallel strong trace can be defined similarly.

Note that the experimentally obtained tetrahedron, TET12, has four parallel and two antiparallel coiled-coil pairs. Viewed as a double trace it has four parallel edges and two antiparallel edges. It has been proved theoretically that such a single-chain tetrahedron cannot be constructed without the use of both parallel and antiparallel pairs [6]. This further motivates us to introduce the following notions.

Let T be a double trace in G and $F \subseteq E$. We say that T is an *F-double trace* of G if edges in $E \setminus F$ are parallel and edges in F are antiparallel with respect to T. Furthermore, T is said to be an *F-strong trace* if T is not only an F-double trace but also a strong trace. Observe that the parallel strong trace and the antiparallel strong trace are both special cases of F-strong trace with $F = \emptyset$ and $F = E$, respectively.

The purpose of this paper is to study, given a graph $G = (V, E)$ and $F \subseteq E$, whether there exists an F-strong trace in G. We solve it when (V, F) is acyclic, by proving that in this case G admits an F-strong trace if and only if $G \setminus F$ is even. We give two examples to show that this condition is not always true when (V, F) contains cycles.

By now more parallel coiled-coil dimers have been characterized for the molecular design than antiparallel dimers [7]. It is therefore more applicable when F has relatively few edges compared with edges of G, including the case that F induces a forest. In [12], the authors studied the cases that F is an independent set or induces a path or cycle. The main result of this paper contains the case that F is an independent set or induces a path.

2 Some known results

A *d-stable trace* is a double trace without repetitions of order i for all $1 \leq i \leq d$. Note that a proper trace (resp. stable trace) is exactly a 1-stable trace (resp. 2-stable trace). It follows from the definitions that we have:

Proposition 2.1 *Let T be a strong trace of G. Then T is a d-stable trace of G if and only if $\delta(G) > d$.*

Let T be a double trace in G, $v \in V$, the *vertex figure* of v of G with respect to T, denoted by $F_{v,T}$, is a 2-regular graph having $E(v)$ as its vertex set and making edges $e, e' \in E(v)$ adjacent if e and e' are consecutive edges along T. The connected components of a vertex figure are cycles, including: a vertex with a loop (C_1) and two vertices connected by two parallel edges (C_2) as special cases. The vertex figure is quite useful in describing strong trace.

Lemma 2.1 *[5] Let T be a double trace in G. Then T is a strong trace if and only if $F_{v,T}$ is connected (i.e. a single cycle) for every $v \in V$.*

The characterization of graphs that admit a proper trace, stable trace, d-stable trace and strong trace were studied in [8,9], [4] and [5], respectively.

Lemma 2.2 *[4, 5, 8, 9]*

(1) A graph G admits a proper trace if and only if $\delta(G) \geq 2$;

(2) A graph G admits a stable trace if and only if $\delta(G) \geq 3$;

(3) A graph G admits a d-stable trace if and only if $\delta(G) > d$;

(4) Every graph admits a strong trace.

The necessary and sufficient conditions of graphs that admit a parallel proper trace [4], parallel stable trace [10], parallel d-stable trace [5] and parallel strong trace [5] were investigated respectively.

Lemma 2.3 *[4, 5, 10]*

(1) A graph G admits a parallel proper trace if and only if G is Eulerian;

(2) A graph G admits a parallel stable trace if and only if G is Eulerian and $\delta(G) \geq 3$;

(3) A graph G admits a parallel d-stable trace if and only if G is Eulerian and $\delta(G) > d$;

(4) A graph G admits a parallel strong trace if and only if G is Eulerian.

In [5], Fijavž, Pisanski and Rus characterized graphs that admit an antiparallel strong trace as follows:

Lemma 2.4 *[5] A graph G admits an antiparallel strong trace if and only if G has a spanning tree ST such that each connected component of $G \setminus E(ST)$ has an even number of edges.*

A graph G that admits an F-double trace was independently characterized by Vastergaard [11] and by Fleischner [1].

Lemma 2.5 *[1, 11] Let G be a connected graph and $F \subseteq E(G)$. G admits an F-double trace if and only if $G \setminus F$ is even.*

3 Our results

Theorem 3.1 *Let $G = (V, E)$ be a connected graph, $F \subset E$ and (V, F) be a forest. Then G admits an F-strong trace if and only if $G \setminus F$ is even.*

By Lemma 2.5, we only need to prove the following lemma.

Lemma 3.1 *Let $G = (V, E)$ be a connected graph, $F \subset E$ and (V, F) be a forest. If $G \setminus F$ is even, then G admits an F-strong trace.*

Proof We prove the lemma by induction on l, the cardinality of F. Lemma 2.3(4) implies the lemma is true for $l = 0$ (and for any G). Now assume that the lemma is true for any F and G with $|F| = l < k$ ($k \geq 1$). Now we suppose that $F \subset E$, $|F| = k$, (V, F) is a forest and $G \setminus F$ is even, we shall prove that G admits an F-strong trace.

Notice that $F \subset E$ and $G \setminus F$ is even, then there must exist an edge of F, say $e = u_1u_2$, such that at least one of its two endpoints is of degree $d \geq 2$ in $G \setminus F$. Without loss of generality, suppose that $d_{G\setminus F}(u_2) \geq 2$. There are two cases.

Case 1 e is not a cut edge of G.

Let $G' = G \setminus e$ and $F' = F \setminus e$. It is obvious that G' is connected, $F' \subset E(G')$, (V, F') is a forest of G' and $G' \setminus F'$ is even since $G' \setminus F' = G \setminus F$. By the induction hypothesis, G' admits an F'-strong trace T'. Moreover, there is at least one edge, say e_2 , such that $e_2 \in E_{G'}(u_2) \setminus F'$, is traversed twice and both towards u_2 along T', since edges in $F' \cap E_{G'}(u_2)$ are all antiparallel edges, keeping in-coming and out-going edges balanced. Note that $d_{G'}(u_1) \geq 1$ and that $d_{G'}(u_2) \geq 2$, without loss of generality, we may describe the strong trace T' as:

$$T' = v_1e_1u_1f_1w_1t_1v_2e_2u_2f_2w_2t_2v_2e_2u_2h_2y_2t_3$$

such that $e_1, f_1 \in E_{G'}(u_1)$ ($e_1 = f_1$ if and only if $d_{G'}(u_1) = 1$), and that $f_2, h_2 \in E_{G'}(u_2)$ ($h_2 = f_2$ if and only if $d_{G'}(u_2) = 2$), moreover, t_1, t_2 and t_3 are segments of T' that e_2 is not contained in t_i for $i \in \{1, 2, 3\}$. See Figure 4(1). Now we construct a new double trace T of G from T' as follows.

$$T = v_1e_1u_1eu_2f_2w_2t_2v_2e_2u_2eu_1f_1w_1t_1v_2e_2u_2h_2y_2t_3.$$

See Figure 4(2). In fact, roughly speaking, T is a double trace of G obtained from T' by interchanging two segments between u_1 and u_2 with direction preserved and by adding the edge e which is traversed exactly once in each direction. Therefore, T is an F-double trace of G.

Next, we shall show that T is a strong trace of G. For $v \notin \{u_1, u_2\}$, its vertex figure $F_{v,T}$ is exactly the same as $F_{v,T'}$, which is a single cycle by Lemma 2.1. For $v = u_i$ ($i = 1, 2$), it is not difficult to see that the vertex figure $F_{u_i,T}$ is obtained from $F_{u_i,T'}$ by replacing the edge e_if_i with two adjacent edges e_ie and ef_i as shown in Figure 5. Hence, $F_{u_i,T}$ is also a single cycle and thus T is an F-strong trace of G.

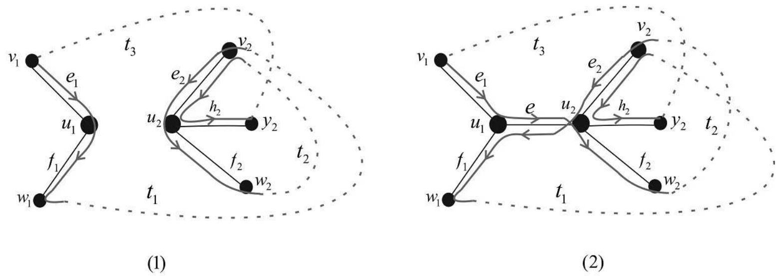


Figure 4. The strong traces: (1) T' and (2) T. Note that, $v_1 = w_1$ if and only if $d_{G'}(u_1) = 1$, and that $y_2 = w_2$ if and only if $d_{G'}(u_2) = 2$.

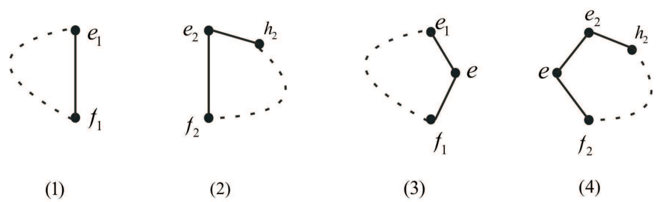


Figure 5. The vertex figures: (1) $F_{u_1,T'}$, (2) $F_{u_2,T'}$, (3) $F_{u_1,T}$, (4) $F_{u_2,T}$.

Case 2 e is a cut edge of G.

Let G_1 and G_2 be two connected components of $G \setminus e$ with $u_i \in V(G_i)$. For $i = 1, 2$, set $F_i = F \cap E(G_i)$. Then $F_i \subseteq E(G_i)$ and (V_i, F_i) is a forest of G_i, and $F_2 \subset E(G_2)$ since $d_{G\setminus F}(u_2) \geq 2$. Now we first prove that G_1 admits an F_1-strong trace T_1. If $F_1 \subset E(G_1)$, then G_1 admits an F_1-strong trace by the induction hypothesis; if $F_1 = E(G_1)$, then G_1 is a tree and admits an F_1-strong trace by Lemma 2.4. Second, G_2 admits an F_2-strong trace T_2 by the induction hypothesis. By the similar arguments of Case 1, there must exist an edge in G_2, say e_2, that is incident with u_2 and is traversed twice towards u_2 in T_2. Without loss of generality, we may describe T_2 as

$$T_2 = v_2 e_2 u_2 f_2 w_2 t_2 v_2 e_2 u_2 h_2 y_2 t_2'$$

such that $f_2, h_2 \in E_{G_2}(u_2)$ ($h_2 = f_2$ if and only if $d_{G_2}(u_2) = 2$), and that t_2 and t_2' are segments of T_2. See Figure 6(2).

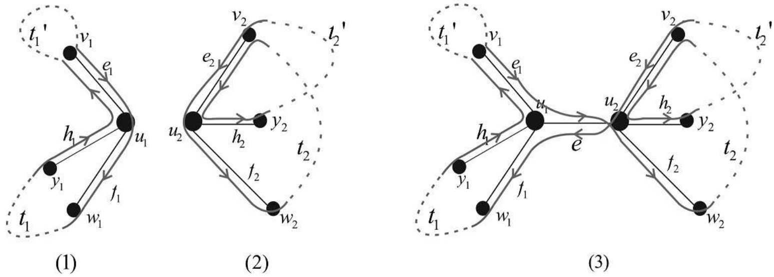


Figure 6. (1) The strong trace T_1, (2) The strong trace T_2, (3) Construct T from T_1 and T_2.

Subcase 2.1 $d_{G_1}(u_1) \geq 2$ and each edge incident with u_1 is traversed exactly once in each direction in T_1. Without loss of generality, we may describe T_1 as

$$T_1 = v_1 e_1 u_1 f_1 w_1 t_1 y_1 h_1 u_1 e_1 v_1 t_1',$$

such that $e_1, f_1, h_1 \in E_{G_1}(u_1)$ ($h_1 = f_1$ if and only if $d_{G_1}(u_1) = 2$), and that t_1 and t_1' are segments of T_1. See Figure 6(1). Now we construct T as follows.

$$T = v_1 e_1 u_1 e u_2 f_2 w_2 t_2 v_2 e_2 u_2 h_2 y_2 t_2' v_2 e_2 u_2 e u_1 f_1 w_1 t_1 y_1 h_1 u_1 e_1 v_1 t_1'.$$

See Figure 6(3). It is clear that T is an F-double trace of G. By the analogous analysis to that of Case 1, each vertex figure $F_{v,T}$ is a single cycle, therefore, T is an F-strong trace of G.

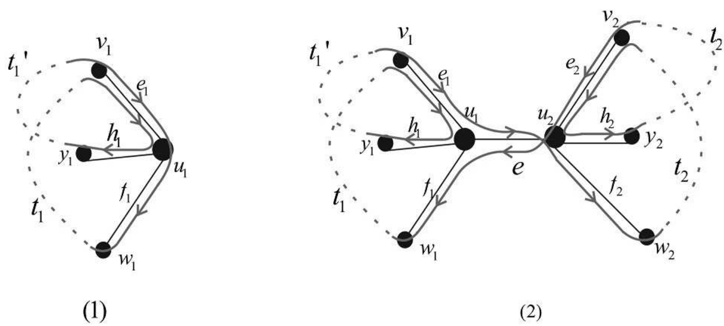


Figure 7. (1) The strong traces T_1, (2) Construct T from T_1 and T_2.

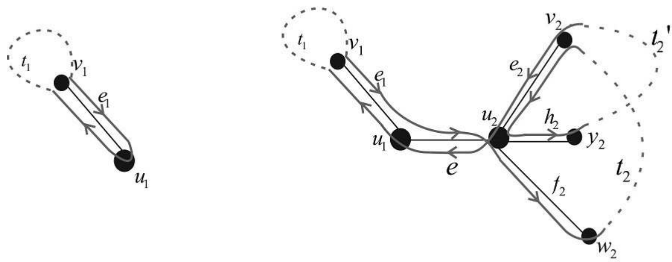
Subcase 2.2 $d_{G_1}(u_1) \geq 2$ and there is at least one edge, say e_1, that is incident with u_1 and is traversed in the same direction in T_1. Without loss of generality, assume that e_1 is traversed twice towards u_1 in T_1. Then we may describe T_1 as

$$T_1 = v_1e_1u_1f_1w_1t_1v_1e_1u_1h_1y_1t_1',$$

such that $f_1, h_1 \in E_{G_1}(u_1)$ ($h_1 = f_1$ if and only if $d_{G_1}(u_1) = 2$), and that t_1 and t_1' are segments of T_1. See Figure 7(1). Construct a double trace T of G as follows:

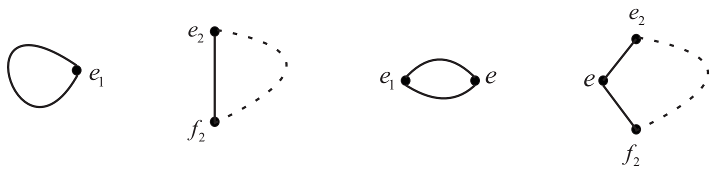
$$T = v_1e_1u_1eu_2f_2w_2t_2v_2e_2u_2h_2y_2t_2'v_2e_2u_2eu_1f_1w_1t_1v_1e_1u_1h_1y_1t_1'.$$

See Figure 7(2). By the similar arguments to that of Subcase 2.1, T is an F-strong trace of G.



(1) (2)

Figure 8. (1) The strong traces T_1, (2) Construct T from T_1 and T_2.



(1) (2) (3) (4)

Figure 9. The vertex figures: (1) F_{u_1,T_1}, (2) F_{u_2,T_2}, (3) $F_{u_1,T}$, (4) $F_{u_2,T}$.

Subcase 2.3 $d_{G_1}(u_1) = 1$. Assume that $E_{G_1}(u_1) = \{e_1\}$, then e_1 must be antiparallel in T_1. Without loss of generality, we may describe T_1 as

$$T_1 = v_1e_1u_1e_1v_1t_1,$$

such that t_1 is a segment of T_1. See Figure 8(1).

Construct T as follows.

$$T = v_1e_1u_1eu_2f_2w_2t_2v_2e_2u_2h_2y_2t_2'v_2e_2u_2eu_1e_1v_1t_1.$$

See Figure 8(2). By the similar arguments to that of Subcase 2.1 and by Figure 9, T is an F-strong trace of G.

Subcase 2.4 $d_{G_1}(u_1) = 0$. Construct T as follows.

$$T = v_2e_2u_2eu_1eu_2f_2w_2t_2v_2e_2u_2h_2y_2t_2'.$$

See Figure 10(1). By Figure 10 and by the analogous arguments to that of Subcase 2.1, T is an F-strong trace of G.

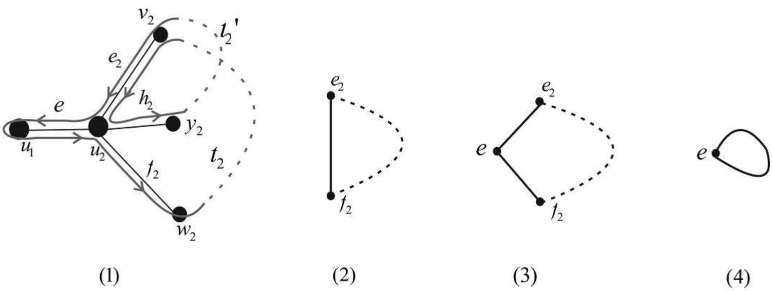


Figure 10. (1) The strong trace T, (2) The vertex figure F_{u_2,T_2}, (3) The vertex figure $F_{u_2,T}$, (4) The vertex figure $F_{u_1,T}$.

This completes the proof of Lemma 3.1. □

As a result of combining Proposition 2.1 with Theorem 3.1, we have:

Corollary 3.1 *Let $G = (V, E)$ be a connected graph, $F \subset E$, (V, F) be a forest of G. Then G admits an F- and d-stable trace if and only if $\delta(G) > d$ and $G \setminus F$ is even.*

4 Concluding remarks

Except Figure 3, two other mathematical topological solutions of self-assembling tetrahedron from a single chain are also given in [6]. See Figure 11. Note that in these two models, the antiparallel edges both form a star with 3 arms. These solutions are consistent with our Theorem 3.1.

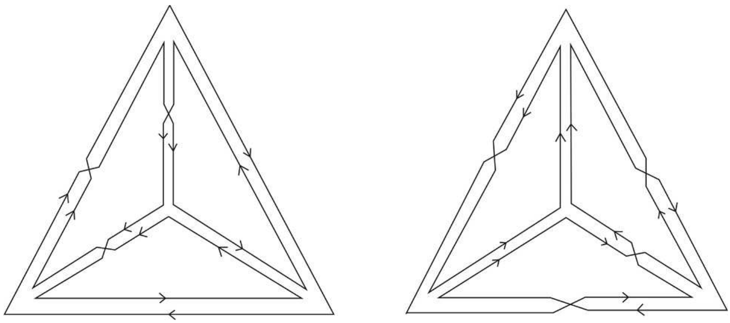


Figure 11. Two other mathematical models of self-assembling tetrahedron from a single chain.

It is proved that if F induces a 2-regular graph (i.e. disjoint union of cycles) and $G \setminus F$ is even then G admits an F-stong trace [12]. Let $F \subset E$. It is then natural to ask that if the condition $G \setminus F$ is even can always guarantee that G has an F-strong trace when (V, F) contains cycles. The answer is "no". Here we give two examples: one has cut edges and the other has not.

Example 4.1 *Let H be the graph depicted in Figure 12, whose vertex set V is $\{u_i, v_i, w_i | i = 1, 2\}$ and edge set E is $\{u_iv_i, u_iw_i, v_iw_i | i = 1, 2\} \cup \{u_1u_2\}$. Let $F = \{u_1u_2, u_1v_1, u_1w_1, v_1w_1\}$, it is seen that (V, F) is not a forest and $H \setminus F$ is even. But H does not admit an F-strong trace.*

Proof Suppose that T is an F-double trace of H, without loss of generality, assume that the edge u_2w_2 is traversed twice from u_2 to w_2 in T, then the directions of w_2v_2 and v_2u_2 must be as shown in Figure 12. Start from an edge of H, say u_1u_2, without loss of generality, assume that it is traversed from u_1 to u_2 firstly, then the second edge must be u_2w_2, otherwise, a retracing occurs at u_2. Since the edge u_1u_2 is a cut edge of H, three edges u_2w_2, w_2v_2 and v_2u_2 must be traversed exactly twice before T goes from u_2 to u_1. We keep going along T, without loss of generality, the successive edge of u_2u_1 is u_1v_1, then the next edges must be v_1w_1 and w_1u_1. Now we can see that a retracing will occur at u_1 and therefore H does not admit an F-strong trace. $\square$

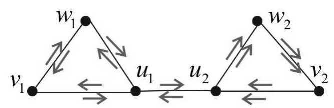


Figure 12. The graph H and orientations.

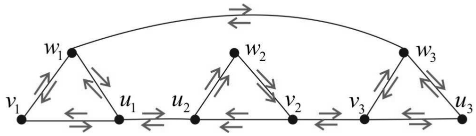


Figure 13. The graph G and orientations.

Example 4.2 *Let G be the graph with vertex set $V = \{u_i, v_i, w_i | i = 1, 2, 3\}$ and edge set $E = \{u_iv_i, u_iw_i, v_iw_i | i = 1, 2, 3\} \cup \{w_1w_3, u_1u_2, v_2v_3\}$ as shown in Figure 13. Let $F = \{u_iv_i, u_iw_i, v_iw_i | i = 1, 3\} \cup \{u_1u_2, v_2v_3, w_1w_3\}$. Then (V, F) is not a forest and $G \setminus F$ is even. But G does not have an F-strong trace.*

Proof Let G_1 be the subgraph of G induced on vertex set $\{u_i, v_i, w_i | i = 1, 2\}$ and $F_1 = F \cap E(G_1)$. Then $G_1 = H$, the graph in Example 4.1. Furthermore, we color the four edges in F_1 yellow and three edges in $E(G_1) \setminus F_1$ blue. Assume to the contrary that G admits an F-strong trace T. Without loss of generality, the orientation of G is as shown in Figure 13. Start from an edge of G, say u_1u_2, without loss of generality, assume that it is traversed from u_1 to u_2 firstly, then the second and third edge must be u_2w_2 and w_2v_2, respectively. Note that the maximum degree of G is 3, in order to avoid retracing and repetition in T, there are at most two possible successive edges when T arrives at a vertex of degree 3, and there is only one possible successive edge when T arrives at a vertex of degree 2. The successive edge of w_2v_2 may be one of v_2v_3 and v_2u_2.

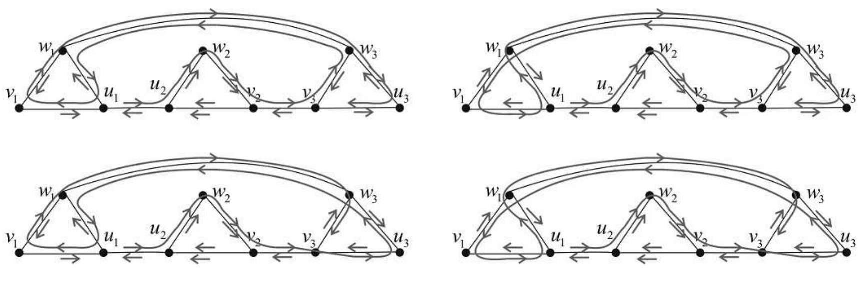


Figure 14. Four possibilities of T if the successive edge of w_2v_2 is v_2v_3.

Case 1 The successive edge of w_2v_2 is v_2v_3. Keep going along T, it will arrive at the vertex w_3 from v_3 either by edge v_3w_3 or by path $v_3u_3w_3$, no matter under which circumstance, the next edge in T must be w_3w_1, otherwise, three blue edges will be traversed twice before T arrives the yellow edges, and an F_1-strong trace of G_1 will be obtained from T by omitting the vertices and edges not in G_1, a contradiction with Example 4.1. By simple analysis, there are four possibilities which are shown in Figure 14. Then a retracing appears at the vertex v_3, a contradiction.

Case 2 The successive edge of w_2v_2 is v_2u_2. We keep going along T, the successive edge of v_2u_2 may be one of u_2w_2 and u_2u_1.

Subcase 2.1 The successive edge of v_2u_2 is u_2w_2. By the similar analysis, there are four possibilities (see Figure 15), in each of which a retracing occurs at vertex v_3, a contradiction.

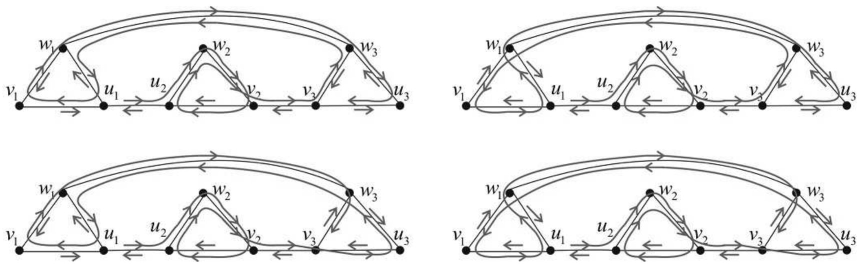


Figure 15. Four possibilities of T if the successive edge of v_2u_2 is u_2w_2.

Subcase 2.2 The successive edge of v_2u_2 is u_2u_1. Then T will arrive at vertex w_1 from u_1 either by edge u_1w_1 or by path $u_1v_1w_1$, no matter how T arrives at w_1, the next edge must be w_1w_3, otherwise, a retracing occurs at u_1. Keep going along T, it will arrive at the vertex v_3 from w_3 either by edge w_3v_3 or by path $w_3u_3v_3$, and the next edge must be v_3v_2 after simple analysis. Thus, there are four possibilities (see Figure 16), in each of

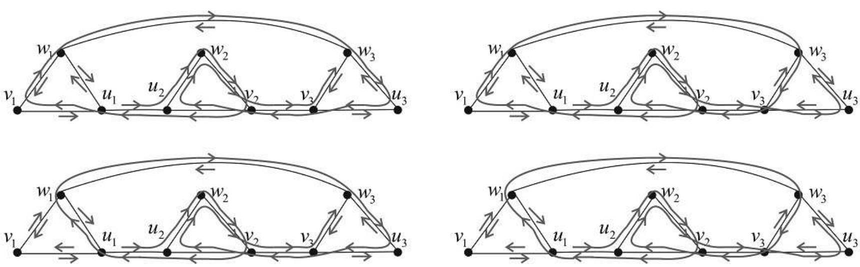


Figure 16. Four possibilities of T if the successive edge of v_2u_2 is u_2u_1.

which a retracing occurs at w_3, a contradiction. □

Finally, Theorem 3.1 can be viewed as a generalization of Lemma 2.3 (4) from $F = \emptyset$ to the F which induces a forest. It is natural to ask if Lemma 2.4 can be extended and which extent can it be extended.

Acknowledgements: We thank Prof. Tomaž Pisanski for his lecture on the 11th meeting of the International Academy of Mathematical Chemistry, which drew our attention to this topic. This work was supported by NSFC (No. 11671336), Hunan Provincial Natural Science Foundation of China (No. 14JJ3138), Hunan Education Department Talent Foundation(No. 16B028) and President's Funds of Xiamen University (No. 20720160011).

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