Applicable Analysis and Discrete Mathematics, **1** (2007), 228–240.
Available electronically at **http://pefmath.etf.bg.ac.yu**

Presented at the conference: *Topics in Mathematical Analysis and Graph Theory*, Belgrade, September 1–4, 2006.

ON UNICYCLIC REFLEXIVE GRAPHS

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A simple graph is said to be reflexive if the second largest eigenvalue of its $(0,1)$-adjacency matrix does not exceed 2. Based on some recent results on reflexive graphs with more cycles and some new observations, we construct in this paper several classes of maximal unicyclic reflexive graphs.

1. INTRODUCTION

If G is a simple graph (a non-oriented graph without loops or multiple edges), its $(0,1)$-adjacency matrix A is symmetric and roots of the *characteristic polynomial* $P_G(\lambda) = \det(\lambda I - A)$ (the *eigenvalues* of G, making up its *spectrum*) are all real numbers, for which we assume their non-increasing order: $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. In a connected graph for the largest eigenvalue λ_1 (the *index* of the graph) $\lambda_1 > \lambda_2$ holds, which need not take place otherwise, since the spectrum of a disconnected graph is the union of spectra of its components. The interrelation between the spectra of a graph and its induced subgraphs is established by the *interlacing theorem*:

Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of a graph G and $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_m$ eigenvalues of its induced subgraph H. Then the inequalities $\lambda_{n-m+i} \leq \mu_i \leq \lambda_i$ $(i = 1, \ldots, m)$ hold.

Thus e.g. if $m = n-1$, $\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2, \ldots$, and also $\lambda_1 > \mu_1$ if G is connected.

Reflexive graphs are graphs having $\lambda_2 \leq 2$. They correspond to some sets of vectors in the Lorentz space $R^{p,1}$ and have some applications to the construction and classification of reflection groups [**7**]. Reflexive graphs that have been investigated so far are trees [**4**], [**6**], some classes of bicyclic graphs [**10**], [**13**] (see also [**8**]) and various classes of cactuses with more than two cycles [**5**], [**9**], [**11**], [**12**].

2000 Mathematics Subject Classification. 05C50.
Key Words and Phrases. Graph theory, second largest eigenvalue, reflexive graph, unicyclic graph.

A *cactus*, or a *treelike graph*, is a graph in which any two cycles have at most one common vertex, i.e. are edge-disjoint. A vertex of a cycle in a cactus is said to be *loaded* if its degree is greater than 2. A cycle of a cactus is a *free cycle* if it has only one vertex of degree greater than 2.

In this paper we consider unicyclic reflexive graphs. According to the interlacing theorem, for any given number A, any graphic property $\lambda_i \leq A$ is a *hereditary* one, i.e. all induced subgraphs preserve this property, and that is why it is natural to present reflexive graphs through sets of *maximal* (connected) graphs, of course inside the considered class.

Graph G is a maximal reflexive graph inside a given class of graphs C if G is reflexive and any extension $G+v$ that belongs to C has $\lambda_2 > 2$.

Some important general and auxiliary facts, which are essential for further investigations, are given in Section 2. The rest of the article is devoted to its aim - the construction of classes of maximal unicyclic reflexive graphs.

2. SOME FORMER, GENERAL AND AUXILIARY RESULTS

Connected graphs that have $\lambda_1 = 2$ are known as *Smith graphs.*

Lemma 1 ([**15**]). *For a simple graph G $\lambda_1(G) \leq 2$ (resp. $\lambda_1(G) < 2$) if and only if each component of G is an induced subgraph (resp. proper induced subgraph) of one of the graphs of Fig. 1, all of which have index equal to 2.*

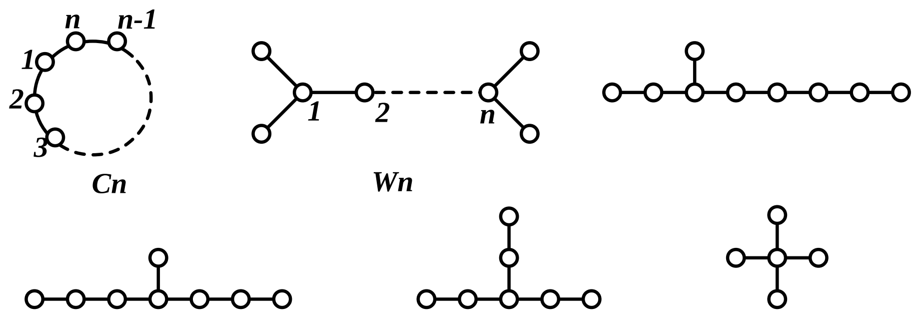

Figure 1.

(In what follows, when saying "subgraph" we will always understand "induced subgraph".)

Lemma 2. ([**14**]). *Given a graph G, let $C(v)$ $(C(uv))$ denote the set of all cycles containing a vertex v and an edge uv of G, respectively. Then*

(i) $P_G(\lambda) = \lambda P_{G-v}(\lambda) - \sum\limits_{u \in \mathrm{Adj}(v)} P_{G-v-u}(\lambda) - 2 \sum\limits_{C \in \mathcal{C}(v)} P_{G-V(C)}(\lambda),$

(ii) $P_G(\lambda) = P_{G-uv}(\lambda) - P_{G-v-u}(\lambda) - 2 \sum\limits_{C \in \mathcal{C}(uv)} P_{G-V(C)}(\lambda),$

where $Adj(v)$ denotes the set of neighbors of v, while $G-V(C)$ is the graph obtained from G by removing the vertices belonging to the cycle C.

These relations have the following consequences (see, e.g. [**1**], p. 59).

Corollary 1. *Let G be a graph obtained by joining a vertex v_1 of a graph G_1 to a vertex v_2 of a graph G_2 by an edge. Let G_1' (G_2') be the subgraph of G_1 (G_2) obtained by deleting the vertex v_1 (v_2) from G_1 (resp. G_2). Then*

$$P_G(\lambda) = P_{G_1}(\lambda)P_{G_2}(\lambda) - P_{G_1'}(\lambda)P_{G_2'}(\lambda).$$

Corollary 2. *Let G be a graph with a pendant edge v_1v_2, v_1 being of degree 1. Then*

$$P_G(\lambda) = \lambda P_{G_1}(\lambda) - P_{G_2}(\lambda),$$

where G_1 (G_2) is the graph obtained from G (resp. G_1) by deleting the vertex v_1 (resp. v_2).

A list of values of $P_G(2)$ for some small graphs is a useful tool in any search for reflexive graphs.

Lemma 3 [**13**]. *Let $G_1, \ldots, G_4$ be the graphs depicted in Fig. 2. Then*

1. $P_{G_1}(2) = k + 2$;
2. $P_{G_2}(2) = 4$;
3. $P_{G_3}(2) = -k\ell m + k + \ell + m + 2$;
4. $P_{G_4}(2) = 4(1 - k\ell)$;

(k, ℓ, m are lengths of corresponding paths).

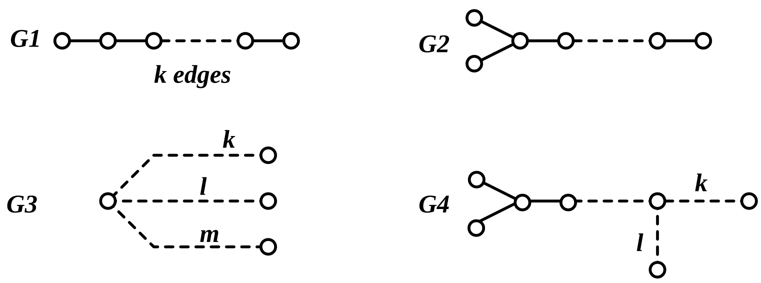

Figure 2.

First supergraphs of Smith graphs have the following property.

Lemma 4 ([**13**]). *Let G be a graph obtained by extending any of Smith graphs by a vertex of arbitrary positive degree. Then $P_G(2) < 0$ (i.e. $\lambda_2(G) < 2 < \lambda_1(G)$).*

The next general theorem can be used to detect a lot of reflexive graphs.

Theorem RS ([**13**]). *Let G be a graph with cut-vertex u.*

(i) *If at least two components of $G - u$ are supergraphs of Smith graphs, and if at least one of them is a proper supergraph, then $\lambda_2(G) > 2$.*

(ii) *If at least two components of* $G - u$ *are Smith graphs, and the rest are subgraphs of Smith graphs, then* $\lambda_2(G) = 2$.

(iii) *If at most one component of* $G - u$ *is a Smith graph, and the rest are proper subgraphs of Smith graphs, then* $\lambda_2(G) < 2$.

This theorem can be applied to a wide class of graphs with a cut-vertex, but if it comes about that $G - u$ consists of one proper supergraph and the rest of proper subgraphs of SMITH graphs, it cannot answer whether the graph is reflexive or not and such cases will be called *RS-indefinite*. In our current investigations we always presuppose that maximal reflexive graphs we are looking for are RS-indefinite.

It turns out that a free cycle in a maximal reflexive cactus can be replaced under some conditions by an arbitrary SMITH tree.

Theorem R (The theorem of replacement) [**10**]. *Suppose that a graph of the form shown in Fig.* 3(a) *is a maximal reflexive cactus for which* $P(2) = 0$ *and* $P_G(2) < 0$ *and for any extension* G_1 *formed by attaching to* G *a pendant edge at any vertex* $P_{G_1}(2) - 2P_{G_1 - v}(2) > 0$ *holds. If the free cycle* C *(of arbitrary length) is replaced by an arbitrary Smith tree* S*, attached to the vertex* v *in an arbitrary way (i.e. at an arbitrary vertex of* S*), then the resulting graph (Fig.* 3(b)) *is again a maximal reflexive cactus.*

If we form a tree T by identifying vertices u_1 and u_2 ($u_1 = u_2 = u$) of two (rooted) trees T_1 and T_2, respectively (the *coalescence* $T_1 \cdot T_2$ of T_1 and T_2), we usually say that T can be *split* at its vertex u into T_1 and T_2 (Fig. 4(a)). Of course, splitting at a given vertex is not determined uniquely if its degree is greater than 2.

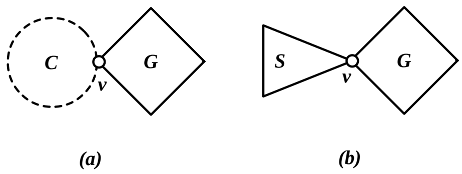

Figure 3.

If we split a tree T at all its vertices in all possible ways, and in each case attach the parts at vertices of splitting u_1 and u_2 to some vertices v_1 and v_2 of a graph G (i.e. lean the parts on G by identifying u_1 with v_1 and u_2 with v_2, and vice versa), we shall say that in the obtained family of graphs the tree T *pours* between v_1 and v_2 (Fig. 4(b)). Of course, this includes attachment of the complete tree T, rooted at any vertex v, to v_1 and v_2. Pouring of SMITH trees turns out to be a very important tool in describing some classes of maximal reflexive graphs ([**5**], [**9**], [**10**], [**12**], [**13**]).

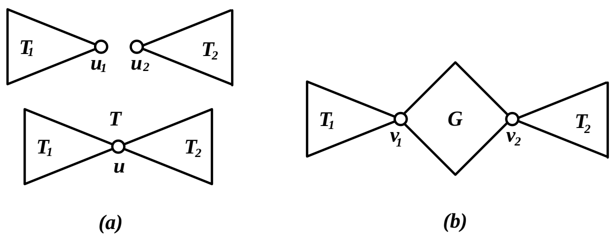

Figure 4.

The result of the next Lemma was already used in [**10**]. Now, we shall formalize the statement.

Lemma 5. *Let a Smith tree S be split at vertex u* $(\deg u > 1)$ *into its subtrees S_1 and S_2 and let us introduce the notation*

$$P_{S_1-u}(2) = p_1, P_{S_2-u}(2) = p_2;$$

$$\sum_{v\in Adj(u)\cap S_1} P_{S_1-u-v}(2) = \Sigma_1, \quad \sum_{v\in Adj(u)\cap S_2} P_{S_2-u-v}(2) = \Sigma_2.$$

Then $\Sigma_1 = \alpha p_1$, $\Sigma_2 = (2-\alpha)\,p_2$, for six different possible values of α.

Proof. If we split W_n into two analogous parts, then $p_1 = \Sigma_1 = p_2 = \Sigma_2 = 4$ and $\alpha = 1$. In the remaining cases one of the two parts S_1, S_2 must be a path, and let it be S_1. We see by an easy calculation based on the application of Lemma 3 that $\Sigma_1 = \alpha p_1$ for $\alpha = \frac{1}{2}, \frac{2}{3}, \frac{3}{4}, \frac{4}{5}, \frac{5}{6}$, depending on whether the path is of length $1, 2, 3, 4, 5$, respectively (and assuming that for a void graph (with no vertices) $P(2) = 1$). Then for all these values of α, $\Sigma_2 = (2-\alpha)\,p_2$ holds, which completes the proof.

3. CLASSES OF MAXIMAL UNICYCLIC REFLEXIVE GRAPHS

Thus far, unicyclic reflexive graphs have not been the subject of any consideration and there are no published results about them. The general problem, to find or describe all such maximal graphs, seems intractable. It is sufficient to have a look at Theorem RS to realize that these graphs can have an arbitrary number of vertices, the cycle can be of arbitrary length, they can have a vertex of arbitrary degree and, after its removal, the remaining graph can have an arbitrary number of components. This means that the investigations should be directed towards specified classes and recent considerations of reflexive graphs with more cycles lead to a number of such classes.

3.1. GRAPHS GENERATED BY MAXIMAL BICYCLIC REFLEXIVE GRAPHS WITH THE BRIDGE BETWEEN THE CYCLES

All maximal reflexive bicyclic graphs whose two cycles are connected by a bridge c_1c_2 were determined in [**13**]. For some practical reasons, in this result a distinction has been made between black vertices of the cycles (those being adjacent to c_1 or c_2) and white vertices (neither black ones nor c_1 or c_2).

Now, based on this result and by applying Theorem R, we can obtain a class of maximal unicyclic reflexive graphs. By inspection of all resulting graphs of [**13**], we see that among those of them that have exactly one free cycle there are those with $\lambda_2 = 2$ as well as others having $\lambda_2 < 2$. One can make sure that the conditions of Theorem R are satisfied always when $\lambda_2 = 2$, and the corresponding unicyclic graphs are displayed in Fig. 5 (all cases with a loaded white vertex) and Fig. 6 (a loaded black vertex , including a case with two loaded black vertices). Clearly, in all these graphs S is an arbitrary Smith tree, rooted at an arbitrary vertex.

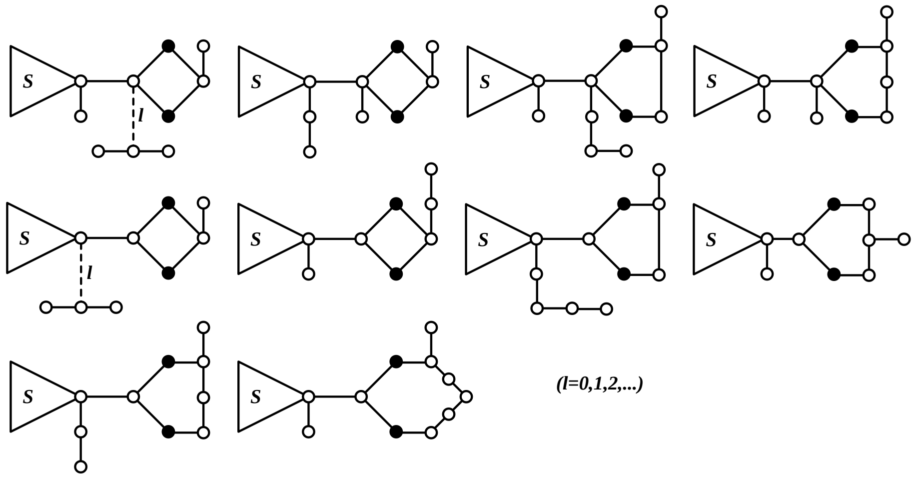

Figure 5.

3.2. POURING OF PAIRS OF SMITH TREES (1)

If we apply Theorem RS to the vertex c_1 of the tricyclic (family of) graphs of Fig. 7(a), we see that $\lambda_2 = 2$, and these graphs are not maximal reflexive graphs since they can be extended at vertices of the free cycle attached to c_1 (bounds of such extensions are just determined by Theorem RS). If we move the other free cycle, e.g. from c_3, to c_2 (Fig. 7(b)), again $\lambda_2 = 2$, but now we have a family of maximal tricyclic reflexive graphs [**13**]. Also, if a Smith tree pours between c_2 and c_3 (Fig. 7(c)), all such graphs are maximal reflexive graphs inside the class of bicyclic graphs with a bridge between the cycles [**13**].

Now, consider the (family of) unicyclic graphs, displayed in Fig. 7(d), where two Smith trees, $S_1 \cdot S_1^{'}$ and $S_2 \cdot S_2^{'}$, pour between the vertices c_2 and c_3. It was established in [**5**] (Lemma 5) that such a graph has $\lambda_2 = 2$ and that any extension by a pendant edge at any vertex of S_1, S_2, $S_1^{'}$ or $S_2^{'}$ implies $\lambda_2 > 2$. In order to construct a class of maximal unicyclic reflexive graphs, we should only examine the possibilities of extension at the vertices of the free cycle attached to c_1.

Theorem 1. *A graph of Fig.* 7(d) *is a maximal unicyclic reflexive graph if and only if it is RS-indefinite, i.e. if and only if the two coalescences at* c_2 *and* c_3 ($S_1 \cdot S_2$ *and* $S_1^{'} \cdot S_2'$) *are not Smith trees.*

Proof. If $S_1 \cdot S_2$, and then consequently $S_1^{'} \cdot S_2^{'}$, are Smith trees, Theorem RS gives $\lambda_2 = 2$ and an extension at the vertices of the cycle is possible up to the boundaries when we get the third Smith tree.

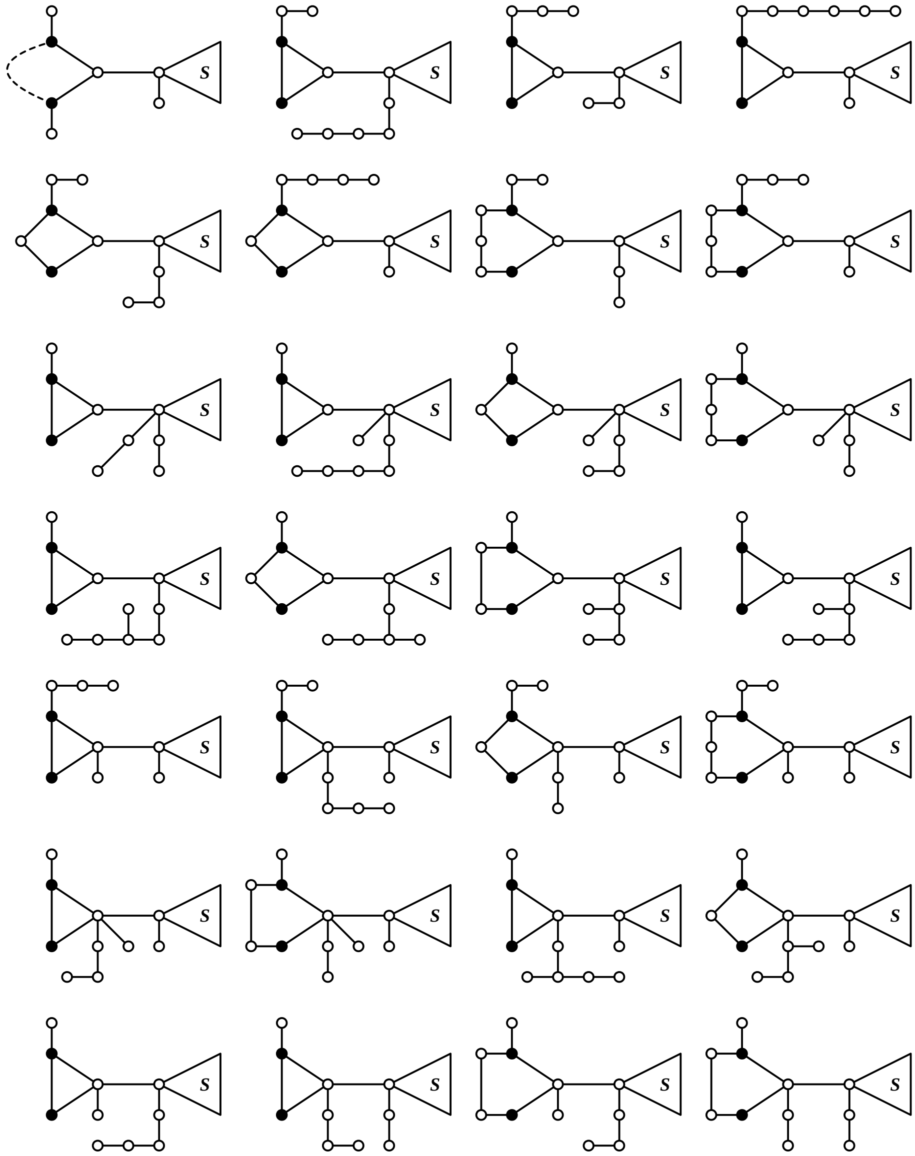

Figure 6.

Suppose now that $S_1 \cdot S_2$ and $S_1^{'} \cdot S_2^{'}$ are not Smith trees, i.e. that one of them, say $S_1 \cdot S_2$ is a proper subgraph of a Smith tree (then $P_{S_1 \cdot S_2}(2) > 0$ holds), and the other a proper supergraph ($P_{S_1' \cdot S_2'}(2) < 0$). If we extend the graph by a pendant edge at the vertex c_1, apply Corollary 2 to this edge and use Lemma 3(1), we get

$$P(2) = 0 - nP_{S_1 \cdot S_2}(2)\, P_{S_1' \cdot S_2'}(2) > 0,$$

which means that such a graph is no more reflexive.

Let us consider now the general case of extension (Fig. 7(e)) and let us introduce the following notation:

$$P_{S_i-c_2}(2)=p_i, P_{S_i'-c_3}(2)=p_i^{'};$$

$$\sum_{v\in S_i\cap Adj(c_2)} P_{S_i-c_2-v}(2)=\Sigma_i, \sum_{v\in S_i^{'}\cap Adj(c_3)} P_{S_i^{'}-c_3-v}(2)=\Sigma_i^{'},$$

where $i=1,2$. According to Lemma 2.(i), for the two coalescences at c_2 and c_3 the following relations hold:

$$\begin{aligned} P_{S_1\cdot S_2}(2) &= 2p_1p_2-p_1\Sigma_2-p_2\Sigma_1,\\ P_{S_1^{'}\cdot S_2^{'}}(2) &= 2p_1^{'}p_2^{'}-p_1^{'}\Sigma_2^{'}-p_2^{'}\Sigma_1^{'}. \end{aligned}$$

Applying now Corollary 2, and then Lemma 2.(i) to (the vertex c_1 of) the remaining graphs, and using also Lemma 3.(1), we obtain:

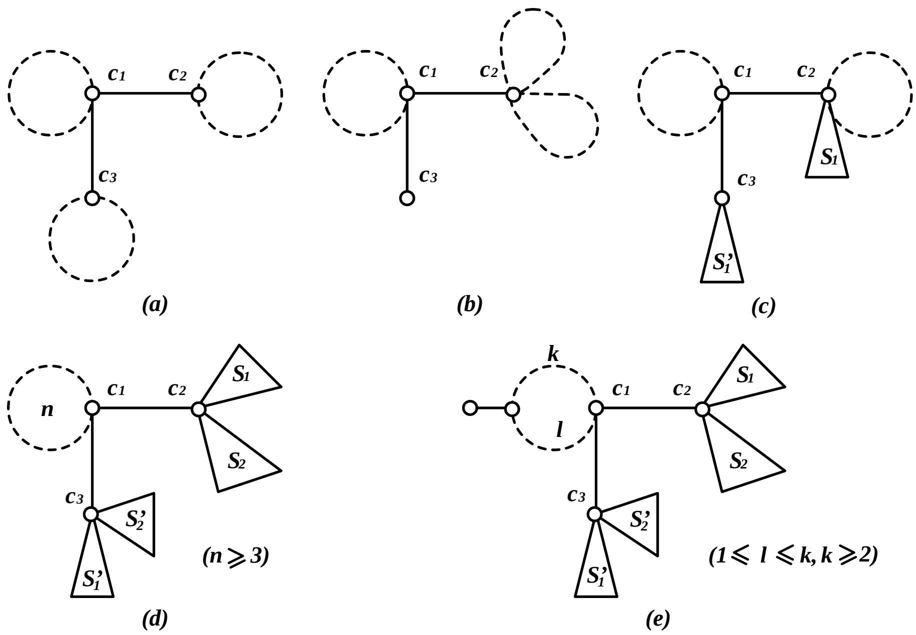

Figure 7.

$$\begin{aligned} P(2) &= 0-(2k\ell-k(\ell-1)-(k-1)\ell)(2p_1p_2-p_1\Sigma_2-p_2\Sigma_1)\cdot\\ &\quad\cdot\Big(2p_1^{'}p_2^{'}-p^{'}\Sigma_2^{'}-p_2^{'}\Sigma_1^{'}\Big)+k\ell\Big(p_1p_2\left(2p_1'p_2'-p_1'\Sigma_2'-p_2'\Sigma_1'\right)\\ &\qquad +p_1'p_2'\left(2p_1p_2-p_1\Sigma_2-p_2\Sigma_1\right)\Big). \end{aligned}$$

Now, according to Lemma 5, $\Sigma_1 = \alpha p_1$, $\Sigma_1' = (2-\alpha)\, p_1'$ and also $\Sigma_2 = \beta p_2$, $\Sigma_2' = (2-\beta)\, p_2'$, which gives

$$P\,(2) = (k+l)\, p_1 p_2 p_1' p_2' \,(\alpha + \beta - 2)^2 \geq 0.$$

Since S_1, S_2, $S_1^{'}$ and $S_2^{'}$ all are parts of Smith trees, it is clear from the list of numbers that appear in the proof of Lemma 5 that, if $S_1 \cdot S_2$ and $S_1' \cdot S_2'$ are not Smith trees, then $\beta \neq 2 - \alpha$ holds. But since $P\,(2) > 0$ means $\lambda_2 > 2$, the extension is not possible and the proof is complete.

3.3. POURING OF PAIRS OF SMITH TREES (2)

If we introduce a new vertex c_4 to the graph of Fig. 7(d), join it to c_2 and c_3, and then attach to c_4 a free cycle (Fig. 8(a)), such a graph still has $\lambda_2 = 2$ and is a maximal tricyclic reflexive graph. It cannot be extended at vertices of two pouring Smith trees because of (the already mentioned) Lemma 5 of [**5**], while any extension at vertices of the free cycles is impossible because the removal of c_2 and application of Theorem RS to c_3 would give $\lambda_2 > 2$.

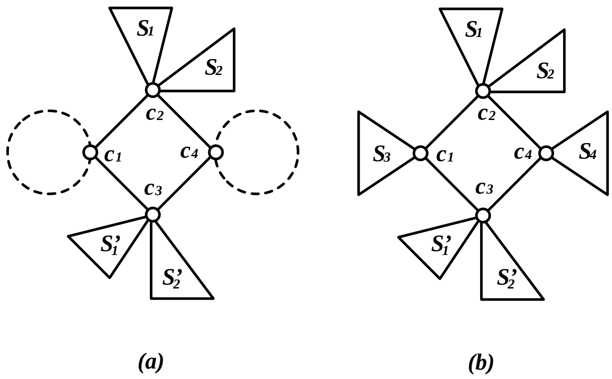

Figure 8.

Can the two free cycles be replaced by two Smith trees S_3 and S_4? In this case Theorem R cannot be applied ($P_G\,(2) < 0$ does not hold).

In the same way as it was done in [**5**], we can verify the fact that a graph obtained by removing c_4 from the case (b) also allows no extension at the vertices of S_i and $S_i^{'}$ $(i = 1, 2)$. As for vertices of S_3 and S_4, no extension is possible for the same reason as at free cycles in the case (a). Thus, if the graph of Fig. 8(b) has $\lambda_2 = 2$, it is a maximal unicyclic reflexive graph. On the other hand, no counter-example ($\lambda_2 > 2$) is known, but the case has to be verified by a computer.

Conjecture. *All graphs of the form of Fig.* 8(b) *have* $\lambda_2 = 2$ *and therefore all of them are maximal unicyclic reflexive graphs.*

3.4. POURING OF TRIPLES OF SMITH TREES

Consider the family of bicyclic graphs in Fig. 9(a): a free cycle is attached to a vertex c_1 of a triangle, while three Smith trees pour between c_2 and c_3. Let p_i and Σ_i $(i = 1, 2, 3)$ have the same meaning as in Theorem 1. According to a result of [**10**], such graphs are maximal bicyclic reflexive graphs, with the following three exceptions:

1) two complete Smith trees are attached to c_2 and c_3, respectively, while the third (pouring) tree is W_n, split into two analogous parts;

2) a complete Smith tree S_1 is attached to, say, c_2, while each of two remaining Smith trees is split into K_2, attached to c_2, and $S_i^{'}$ $(i = 2, 3)$, attached to c_3;

3) for one of the two coalescences of three parts of three pouring Smith trees, say S_1, S_2, S_3, there exist corresponding parts $\bar{S}_1$, $\bar{S}_2$, $\bar{S}_3$ such that S_i and $\bar{S}_i$ $(i = 1, 2, 3)$ have the same values p_i and Σ_i (i.e. belong to the same one of the six classes described in Lemma 5), which, of course, includes the possibility $S_i = \bar{S}_i$ for some i, and such that the analogous coalescence generated by $\bar{S}_1$, $\bar{S}_2$ and $\bar{S}_3$ consists of a complete Smith tree and two additional pendant edges (as in case(2)).

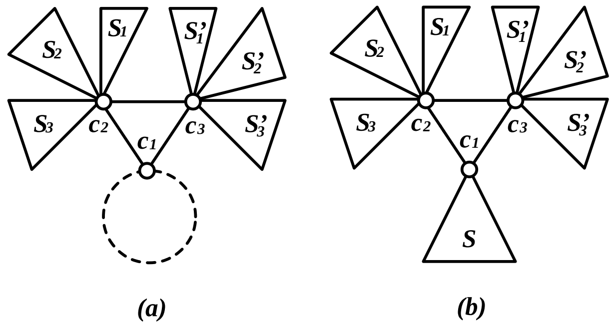

Figure 9.

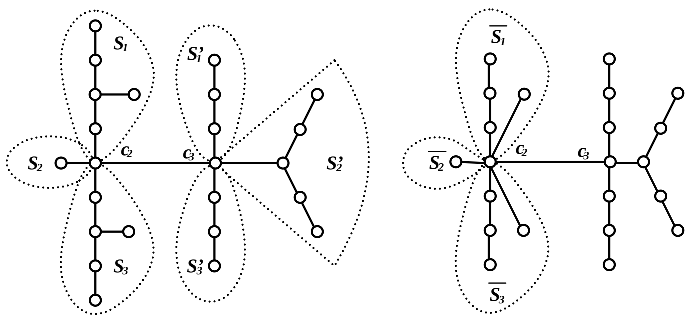

Figure 10.

The graphs of Fig. 10 illustrate the description of case (3).

In these three cases graphs of Fig. 9(a) are not maximal and can be extended at some vertices of the cycle attached to c_1; the resulting maximal graphs are also found in [**10**], and the same family of exceptional maximal graphs appears in all three exceptional cases described above.

Based on the analysis which led to this result of [**10**] (the removal of c_1 and the application of Corollary 1 to the bridge c_2c_3 may give $P(2) < 0$ or $P(2) = 0$), one can make sure that the theorem of replacement (Theorem R) can apply to graphs of Fig. 9(a) and generate those of Fig 9(b) except exactly in the three exceptional cases. On the other hand, if some of these three cases occurs, replacement of the free cycle by Smith trees gives graphs that are not maximal and allow further extensions. Finding maximal graphs in these cases requires additional investigation.

Theorem 2. *Let a graph G consist of a triangle, a Smith tree S attached (in an arbitrary way) to its vertex c_1, and let a triple of Smith trees pour between the remaining two vertices c_2 and c_3 (Fig.* 9(b)*). If G is none of the three exceptional cases, described above, then G is a maximal unicyclic reflexive graph.*

3.5. MAXIMUM NUMBER OF LOADED VERTICES

As we have seen, the cycle of a maximal unicyclic reflexive graph need not have more than one loaded vertex. We are going now to examine the case of maximum number of loaded vertices.

Theorem 3. *The cycle of unicyclic reflexive graph of length greater than* 8 *cannot have more than* 7 *loaded vertices.*

Proof. In C_9 (the cycle of length 9) one can verify by direct calculation that there cannot be 8 loaded vertices.

Let now the length of the cycle be at least 10 and suppose that it has two vertices, u and v, such that, after deleting them, each component contains at least 4 loaded vertices. In this case each such component is a proper supergraph of W_n, and, according to Theorem RS, $\lambda_2 > 2$.

If such vertices u and v do not exist, then on the cycle there must be $8, 7, 6$ or 5 consecutive loaded vertices, or loaded vertices must be grouped in 3 sets of consecutive vertices of the form $3 + 3 + 2$.

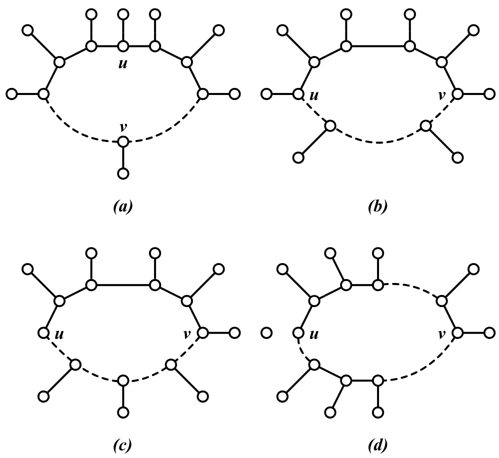

Figure 11.

Case 1 (8 consecutive vertices): if we delete all other (non-loaded) vertices of the cycle, the remaining graph has $\lambda_2 > 2$.

Case 2 (7 vertices): after deleting the two vertices u and v in Fig. 11(a), we obtain two proper supergraphs of W_n.

Case 3 (6 vertices): the deletion of the two vertices u and v in Fig. 11(b) gives rise to two supergraphs of W_n, at least one of them being proper.

Case 4 (5 vertices): as in previous cases, we get two proper supergraphs of W_n (Fig. 11(c)).

Case 5 (3+3+2): now the cycle is at least C_{11} and we again have two proper supergraphs of W_n (Fig. 11(d)).

The proof is complete.

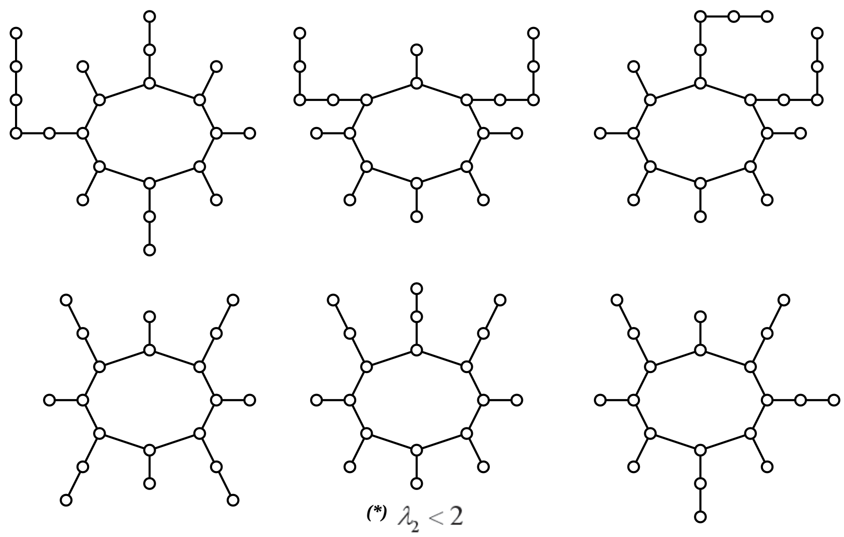

Figure 12.

However, C_8 can have all the vertices loaded and direct checking shows that there are six such cases.

Theorem 4. *The maximum number of loaded vertices of the cycle of a maximal unicyclic reflexive graph is* 8. *There are six such graphs and they are displayed in Fig.* 12.

Acknowledgement: The work on this article has been facilitated by using the programming package GRAPH [**2**].

Also, the author is grateful to the Serbian Ministry of Science and Environment Protection for financial support.

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(Received November 3, 2006)