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ON INVERTIBLE NON-BIPARTITE UNICYCLIC GRAPHS WITH A UNIQUE PERFECT MATCHING AND THEIR SMALLEST POSITIVE EIGENVALUES[*]

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Abstract. Let G be a simple connected graph with the adjacency matrix $A(G)$. By the smallest positive eigenvalue of G, we mean the smallest positive eigenvalue of $A(G)$ and denote it by $\tau(G)$. Recently, the smallest positive eigenvalue of bipartite unicyclic graphs with a unique perfect matching has been studied, and the extremal graphs having the minimum and the maximum τ values have been characterized. We consider the same problem for non-bipartite case. A graph G is said to be positively invertible (respectively, negatively invertible) if there exists a signature matrix S such that $SA(G)^{-1}S$ is nonnegative (respectively, nonpositive). In [S. Akbari and S.J. Kirkland. On unimodular graphs. Linear Algebra Appl., 421:3–15, 2007], the authors characterized all the bipartite unicyclic graphs with a unique perfect matching that are positively invertible. In this article, we characterize all the non-bipartite unicyclic graphs with a unique perfect matching that are positively invertible and negatively invertible, respectively. As an application, we obtain the unique graph with the minimum τ among all the non-bipartite unicyclic graphs on n vertices with a unique perfect matching. Except for a specific class, we characterize all other non-bipartite unicyclic graphs G with a unique perfect matching such that $\tau(G) < \frac{1}{2}$. Further, we show that if G is a non-bipartite unicyclic graph with a unique perfect matching, then $\tau(G) \leq \frac{\sqrt{5}-1}{2}$. The extremal graphs with $\tau = \frac{\sqrt{5}-1}{2}$ have been obtained. Finally, we obtain the graphs with the maximum τ among all the non-bipartite unicyclic graphs on n vertices with a unique perfect matching.

Key words. Unicyclic graph, Unique perfect matching, Graph inverse, Invertible graph, Smallest positive eigenvalue.

AMS subject classifications. 05C50, 05C05, 05C35, 92E10.

1. Introduction.

Let $G = (V(G), E(G))$ be a simple connected graph with the vertex set $V(G) = \{1, \ldots, n\}$ and the edge set $E(G)$. If two vertices i and j are adjacent in G, we denote it by $i \sim j$ and say $\{i, j\} \in E(G)$. Let $A(G)$ be the adjacency matrix of G. Since $A(G)$ is a real symmetric matrix, all its eigenvalues are real. Let $\lambda_1(G) \leq \lambda_2(G) \leq \cdots \leq \lambda_n(G)$ be the eigenvalues of $A(G)$. The terms singularity, eigenvalues, and the characteristic polynomial of G mean those of $A(G)$. The largest eigenvalue of G is called the *spectral radius* of G and is denoted by $\rho(G)$. We denote the *smallest positive eigenvalue* of G by $\tau(G)$. A *perfect matching* in a graph G is a collection of vertex disjoint edges that covers every vertex of G. Note that a connected graph with a unique perfect matching has even number of vertices and it is nonsingular. A tree is nonsingular if and only if it has a unique perfect matching.

The study of graph inverse was first initiated by Godsil [9]. A nonsingular graph G is said to have an *inverse* if there exists a signature matrix S (a diagonal matrix whose diagonal entries are 1 or -1) such that $S^{-1}A(G)^{-1}S$ is nonnegative. Note that $S^{-1} = S$. In this case, we say that $A(G)^{-1}$ is *signable*, G is *positively invertible* or shortly *invertible*, and the weighted graph associated with $SA(G)^{-1}S$ is called the *inverse graph* of G (denoted by $\mathbf{G}^+$). An invertible graph G is said to be a *self-inverse* graph if G is isomorphic to $\mathbf{G}^+$. If $\mathbf{G}^+$ exists for a graph G, then $\rho(\mathbf{G}^+) = \frac{1}{\tau(G)}$.

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Let G^+ be the weighted graph associated with the matrix $B = A(G)^{-1} = [b_{ij}]$ defined as follows: the vertex set of G^+ is same as that of G and $\{i, j\}$ is an edge with the weight b_{ij} if and only if $b_{ij} \neq 0$. Note that, if G is invertible, then $A(G^+)$ is diagonally similar to $A(\mathbf{G}^+)$. In contrast to the positively invertible graphs, Pavlíková and Ševćović [19] introduced the negatively invertible graphs and presented a lower bound for the smallest positive eigenvalue within a specific class of graphs. A graph G is said to be *negatively invertible* if $A(G)^{-1}$ is signature similar to a nonpositive matrix. To have an in-depth knowledge of graph inverse, we recommend the following articles: [1, 3, 9, 14, 17, 19, 20, 22, 23].

In 1985, Godsil [9] proved that the nonsingular trees are (positively) invertible. In the same paper, he posed the question of characterizing all the bipartite graphs with a unique perfect matching that are (positively) invertible. In 2007, Akbari and Kirkland [1] characterized all (positively) invertible bipartite unicyclic graphs with a unique perfect matching. Later, Yang and Ye [22] provided a complete characterization of (positively) invertible bipartite graphs with a unique perfect matching. Graph inverse is an important tool for studying the smallest positive eigenvalue of nonsingular graphs. Here, we study the invertibility of non-bipartite unicyclic graphs that will be used to extremize the smallest positive eigenvalue. Let $\mathcal{U}_n$ be the class of all connected non-bipartite unicyclic graphs with a unique perfect matching on $n = 2m$ vertices and $\mathcal{U}$ be the class of all connected non-bipartite unicyclic graphs with a unique perfect matching. The following questions arise naturally. (1) Which graphs in $\mathcal{U}_n$ are positively invertible? (2) Which graphs in $\mathcal{U}_n$ are negatively invertible? In [14], Kalita and Sarma studied a class of non-bipartite unicyclic graphs with a unique perfect matching, which are negatively invertible referring by a different name (see [14], Theorem 3.14). We characterize and distinguish the graph classes in $\mathcal{U}_n$ that are positively invertible and negatively invertible, respectively.

The smallest positive eigenvalue of a graph plays an important role in chemical graph theory, in particular in the Hückel molecular orbital (HMO) theory. In HMO theory, a hydrocarbon is represented by a graph known as a *molecular graph*, where the vertices correspond to carbon atoms and the edges represent the bonds between the carbon atoms. The HMO method is a methodology to determine the energies of molecular orbitals of π-electrons (see [8]). Among the numerous π-electron properties that find direct representation through graph eigenvalues, some of the most noteworthy are the total π-electron energy, the energy of the highest occupied molecular orbital (HOMO), the energy of the lowest unoccupied molecular orbital (LUMO), and the separation between HOMO and LUMO, commonly termed as the HOMO-LUMO gap. Interestingly, all these parameters of a molecule are directly related to the smallest positive eigenvalue of the corresponding molecular graph. The *HOMO energy, LUMO energy*, and *HOMO-LUMO gap* in a molecule are approximately equal to the smallest positive eigenvalue, the largest negative eigenvalue, and their difference, respectively, of the corresponding molecular graph. For some more information, see [8, 11, 15]. Another parameter is the *HOMO-LUMO radius* or *HL-index* of a molecular graph G, which is defined as the maximum among the moduli of two median eigenvalues of the graph; see [13].

According to HMO theory, the first ionization potential of a molecule is equal to the negative of the HOMO energy, the first electron affinity of a molecule is equal to the negative of the LUMO energy, and the excitation energy of the lowest electronic transition, corresponding to the HOMO-LUMO jump, is related to the HOMO-LUMO gap; see [16]. The HOMO-LUMO gap of a molecule is related to the kinetic stability. A larger HOMO-LUMO gap indicates higher kinetic stability and lower chemical reactivity; see [10]. This provides additional motivation to study the smallest positive eigenvalue of a graph.

Note that all the graphs considered in this article are with a unique perfect matching, unless otherwise specified. Hence, n is even. We take $n = 2m$. In [9], using the inverse of nonsingular trees, Godsil proved that among all the nonsingular trees on $2m$ vertices, P_{2m} (the path graph on $2m$ vertices) attains the minimum τ. Let us take the path $P_{2m} = [1, 2, \ldots, m, m+1, \ldots, 2m]$, $m \geq 4$. If m is even, let U_e^{2m} be the graph obtained from P_{2m} by adding an edge between the vertices $m-2$ and $m+3$. If m is odd, let U_o^{2m} be the graph obtained from the path P_{2m} by adding an edge between the vertices $m-3$ and $m+2$. In [5], Barik and Behera proved that the unique graph U_e^{2m} (respectively, U_o^{2m}) has the minimum τ among all bipartite unicyclic graphs on $2m$ ($m \geq 4$) vertices with a unique perfect matching when m is even (respectively, when m is odd).

A *corona tree* of a tree T, denoted by $\hat{T}$, is the tree obtained from T by adding a new pendant vertex (degree one) at each vertex of T. In [18], Pavlíková and Krč-Jediný proved that in the class of nonsingular trees on $2m$ vertices, $\hat{P}_m$ (also known as the comb graph on $2m$ vertices) has the maximum τ value. Let us take the path $P_{m-1} = [1, 2, \ldots, m-1]$, $m \geq 3$ and consider the corona tree $\hat{P}_{m-1}$ on $2(m-1)$ vertices. If m is odd, then add two new pendant vertices to $\hat{P}_{m-1}$, one at the vertex $\frac{m-1}{2}$ and one at the vertex $\frac{m+1}{2}$, and then add an edge between them. The resulting graph is a unicyclic graph on $2m$ vertices. Let us name it as $\overline{U}_o^{2m}$. Similarly, if m is even, then add two new pendant vertices to $\hat{P}_{m-1}$, one at the vertex $\frac{m-2}{2}$ and one at the vertex $\frac{m}{2}$, and then add an edge between them. Let us name it as $\overline{U}_e^{2m}$. In [6], Barik and Behera proved that the unique graph $\overline{U}_o^{2m}$ (respectively, $\overline{U}_e^{2m}$) has the maximum τ among all the bipartite unicyclic graphs on $2m$ vertices with a unique perfect matching when m is odd (respectively, when m is even).

The smallest positive eigenvalue of bipartite graphs with a unique perfect matching has been studied by Barik, Behera, and Pati in [7]. Let G'_{2m} be the bipartite graph on $2m$ vertices with the adjacency matrix $A(G'_{2m}) = \begin{bmatrix} \mathbf{0} & B \\ B^T & \mathbf{0} \end{bmatrix}$, where B is the $m \times m$ lower triangular $(0,1)$-matrix with $\frac{m^2+m}{2}$ nonzero entries. It was proved that G'_{2m} has the maximum τ among all the bipartite graphs on $2m$ vertices with a unique perfect matching.

Although most of the chemical graphs are bipartite, there are also several non-bipartite chemical graphs. Fulvene is one such example (see Fig. 1). The corresponding chemical graph is unicyclic, non-bipartite, and with a unique perfect matching. Hence, it is also important to study smallest positive eigenvalue of non-bipartite graphs.

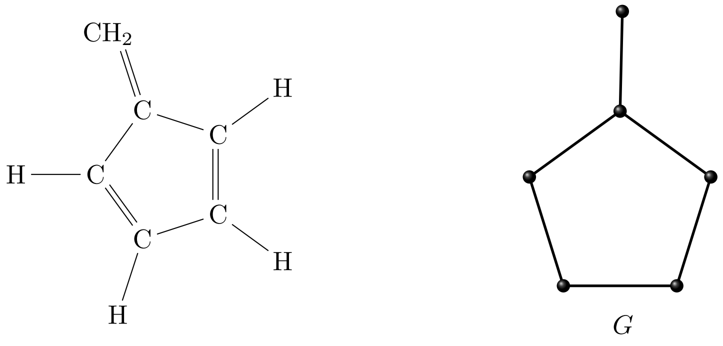

FIGURE 1. *Fulvene (left) and corresponding chemical graph G (right).*

The smallest positive eigenvalue of non-bipartite graphs is not yet studied. For the non-bipartite unicyclic graphs with a unique perfect matching, we consider the following questions. (1) Which graphs in $\mathcal{U}_n$ attain the minimum τ? (2) Which graphs in $\mathcal{U}_n$ attain the maximum τ? Further, looking for upper and lower bounds on τ in the class $\mathcal{U}$ is also interesting for us.

In this article, we characterize the unique graph with the minimum τ among all the graphs in $\mathcal{U}_n$. Let $\tilde{U}_n$ be the unicyclic graph obtained from $P_n = [1, 2, \ldots, n]$, $n \geq 4$ by adding an edge between the vertices 1 and 3. We prove that $\tau(\tilde{U}_n) \leq \tau(U)$ for all $U \in \mathcal{U}_n$.

In [21], Wu et al. proved that if G is a bipartite graph with a unique perfect matching, then $\tau(G) \leq 1$. In [5], the authors provided characterizations of all nonsingular trees T as well as all unicyclic bipartite graphs G with a unique perfect matching having $\tau(G) < \frac{1}{2}$. Using the graph inverse techniques, we characterize all the non-bipartite unicyclic graphs G with a unique perfect matching such that $\tau(G) < \frac{1}{2}$, except for a specific class $\mathcal{U}^*$ (see Definition 4.4). As a consequence, we obtain all the graphs in $\mathcal{U}_n$ with the maximum τ. Further, we prove that if $U \in \mathcal{U}$, then $\tau(U) \leq \frac{\sqrt{5}-1}{2}$. We also characterize the graphs $U \in \mathcal{U}$ such that $\tau(U) = \frac{\sqrt{5}-1}{2}$.

The article is organized as follows. Section 2 contains some definitions and known results. In Section 3, we provide a necessary and sufficient condition for a graph $U \in \mathcal{U}_n$ to be positively invertible (respectively, negatively invertible), and then we characterize the unique graph in $\mathcal{U}_n$ having the minimum τ. In Section 4, we find the graphs in $\mathcal{U}_n$ having the maximum τ. Also, we provide an upper bound on $\tau(U)$ for $U \in \mathcal{U}$ and obtain the extremal graphs.

The following notations are used in this article. By P_n and C_n, we denote the path and cycle on n vertices, respectively. Given a subgraph H of G, by $G - H$ we denote the subgraph of G induced by the vertex set $V(G) \setminus V(H)$. When H is a singleton vertex u, we write $G - H$ as $G - u$. The zero matrix is denoted by O. By E_{ij}, we denote the matrix whose ij-th entry is 1 and all other entries are 0. We use MATLAB software to compute the eigenvalues of some graphs with a small number of vertices. For most of the graphs drawn in this article, the solid lines represent the matching edges and the dotted lines represent the non-matching edges.

2. Preliminaries.

Let A be an $n \times n$ symmetric matrix and B be an $m \times m$ principal submatrix of A. Let $\lambda_1(A) \leq \lambda_2(A) \leq \cdots \leq \lambda_n(A)$ be the eigenvalues of A and $\lambda_1(B) \leq \lambda_2(B) \leq \cdots \leq \lambda_m(B)$ be the eigenvalues of B. The following result (interlacing theorem) finds a relation between the eigenvalues of A and B.

Theorem 2.1. ([12], Theorem 4.3.28) *Let B be a principal submatrix of a symmetric matrix A. Then $\lambda_i(A) \leq \lambda_i(B) \leq \lambda_{n-m+i}(A)$, for $i = 1, \ldots, m$.*

Let $M_n(\mathbb{C})$ denote the set of all $n \times n$ matrices with complex entries. For $A = [a_{ij}] \in M_n(\mathbb{C})$, let $\rho(A)$ denote the spectral radius of A and $|A| = [|a_{ij}|]$.

If a real matrix A is nonnegative, we denote it by $A \geq 0$. For two real matrices A and B, we write $A \geq B$ if $A - B \geq 0$. The following fundamental results on the spectral radius of matrices can be found in [12].

Theorem 2.2. ([12], Theorem 8.1.18) *Let A and B be two $n \times n$ real matrices. If $|A| \leq B$, then $\rho(A) \leq \rho(|A|) \leq \rho(B)$.*

Theorem 2.3. ([12], Theorem 8.4.5) *Let $A, B \in M_n(\mathbb{C})$. Suppose that A is nonnegative, irreducible, and $A \geq |B|$. Let $\lambda = e^{i\phi}\rho(B)$ be a given maximum-modulus eigenvalue of B. If $\rho(A) = \rho(B)$, then there is a diagonal unitary matrix $D \in M_n(\mathbb{C})$ such that $B = e^{i\phi}DAD^{-1}$.*

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The following result about the inverse of a block matrix involving the Schur complements is well known and can be found in [2] and [12].

Lemma 2.4. *Let* $M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ *be a block matrix, where* A *and* D *are square matrices and* D *is invertible. Then,* M *is invertible if and only if the Schur complement* $M_D = A - BD^{-1}C$ *of* D *is invertible. Moreover,*

$$M^{-1} = \begin{bmatrix} M_D^{-1} & -M_D^{-1}BD^{-1} \\ -D^{-1}CM_D^{-1} & D^{-1} + D^{-1}CM_D^{-1}BD^{-1} \end{bmatrix}.$$

Let U be a unicyclic graph with a unique perfect matching $\mathcal{M}$ and Γ be the unique cycle in U. An edge $\{u, v\}$ of U is called a *peg* if $\{u, v\} \in \mathcal{M}$, and it is incident with exactly one vertex of the cycle Γ. Let $p(U)$ denote the number of pegs in U and $g(U)$ denote the number of edges in Γ (girth of U). If $\{u, v\}$ is a peg in U, then we always assume that the vertex v is in the cycle Γ and u is not in Γ. A path P is said to be an alternating path if the edges of it alternate between the edges in $\mathcal{M}$ and those not in $\mathcal{M}$. If the terminating edges of an alternating path are in $\mathcal{M}$, then we say that the path is an *mm*-alternating path. An alternating path is called an *mn*-alternating path if one terminating edge is a matching edge and the other is not. The following is an useful observation.

Observation 2.5. *Let* U *be a unicyclic graph with a unique perfect matching. Then, the following statements hold.*

(i) *There are at most two mm-alternating paths between any two vertices in* U.
(ii) *If* U *is non-bipartite then* $p(U)$ *is odd, and there is at most one alternating path of the same type between any two vertices in* U.

We say a graph G is a *mixed graph*, if it has both directed and undirected edges. If G is a mixed graph, then $A(G)$ is a $(0, 1, -1)$ matrix; see [14]. A spanning subgraph H of a graph G is called a *spanning elementary subgraph* if each component of H is either a cycle or an edge. If H is a spanning elementary subgraph of G, then by $|C_H|$ we denote the number of components in H that are cycles. Let $\mathcal{P}_{ij}$ denote the set of all i-j paths P in G such that $G - P$ has a spanning elementary subgraph. Let U be a non-bipartite unicyclic graph with a unique perfect matching. The following result describes the entries of $A(U)^{-1}$.

Theorem 2.6. (Kalita and Sarma [14], Lemma 3.2) *Let* U *be a non-bipartite unicyclic graph with a unique perfect matching. Then* $A(U)$ *is nonsingular and for* $i \neq j$ *the* ij*-th entry* α_{ij} *of the matrix* $A(U)^{-1}$ *is given by*

$$\alpha_{ij} = \begin{cases} (-1)^{|C_H|+|E(H)|+|E(P)|+|\mathcal{M}|} \; 2^{|C_H|}, & \text{if } |\mathcal{P}_{ij}| = 1; \\ 0, & \text{if } \mathcal{P}_{ij} = \phi, \end{cases}$$

where $P \in \mathcal{P}_{ij}$ *and* H *is the spanning elementary subgraph of* $U - P$*. Furthermore,* $\alpha_{ii} = 0$ *or* ± 2.

The following result has been proved [14].

Theorem 2.7. (Kalita and Sarma [14], Theorem 3.10) *Let* U *be a non-bipartite unicyclic graph with a unique perfect matching and* Γ *be the unique cycle in* U*. Then,* U^+ *is a mixed graph if and only if* U *has at least three pegs.*

Let G be a graph. The *corona* of G, denoted as $\hat{G}$, is defined as the graph obtained from G by adding a new pendant vertex to every vertex of G. The following result is proved in [4].

Theorem 2.8. (Barik, Pati, and Sarma [4]) *Suppose that* G_1 *is a connected graph with* $n \geq 4$ *vertices and* $G = \hat{G}_1$. *If* $\lambda_1(G_1) \leq \lambda_2(G_1) \leq \cdots \leq \lambda_n(G_1)$ *are the eigenvalues of* G_1, *then the eigenvalues of* G *are*

$$\frac{\lambda_i(G_1) \pm \sqrt{\lambda_i(G_1)^2+4}}{2},\ i = 1, \dots, n.$$

3. Non-bipartite unicyclic graphs with a unique perfect matching having minimum τ.

Let U be a non-bipartite unicyclic graph with a unique perfect matching $\mathcal{M}$ and Γ be the unique cycle in U. Assume that α_{ij} is the ij-th entry of $A(U)^{-1}$. From Theorem 2.6, it is clear that if $i \neq j$ and $\alpha_{ij} \neq 0$, then there must exist exactly one path P between i and j such that $U - P$ has a spanning elementary subgraph. Note that if $\alpha_{ij} = \pm 1$, then the path P is an mm-alternating path containing at least one vertex of Γ; see for example the graph U_1 in Fig. 2. If $\alpha_{ij} = \pm 2$, then $U - P$ has a spanning elementary subgraph that contains Γ as one component. Thus, P must be contained in a tree branch that has an odd number of vertices, and other tree branches of U must have an even number of vertices. Furthermore, P is either an mn-alternating path or P contains a vertex k such that both i-k and k-j paths are mn-alternating paths; see for example the graph U_2 in Fig. 2. Notice that, in this case P has equal number of matching and non-matching edges.

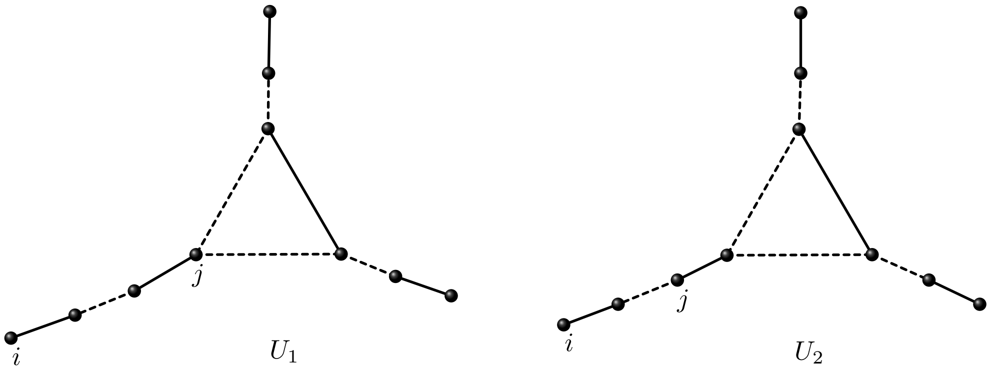

Figure 2. *Examples of non-bipartite unicyclic graphs with a unique perfect matching having exactly one peg.*

Kalita and Sarma [14] characterized the unicyclic graphs G with a unique perfect matching when G^+ is mixed and quasi-bipartite. Note that, if G^+ is quasi-bipartite, then G is negatively invertible. Our next result gives a necessary and sufficient condition for a non-bipartite unicyclic graph with a unique perfect matching to be either positively or negatively invertible.

Theorem 3.1. *Let* U *be a non-bipartite unicyclic graph on vertices* $1, \dots, 2m$, $m \geq 2$ *with a unique perfect matching* $\mathcal{M}$. *Let* Γ *be the unique cycle in* U *and* d *be the number of edges in* Γ *that are in* $\mathcal{M}$. *Then, the following statements hold.*

- (i) *If* d *is odd, then* U *is positively invertible.*
- (ii) *If* d *is even, then* U *is negatively invertible.*

Proof. (i) Let d be odd. To prove that U is positively invertible, we need to find a signature matrix S such that $SA(U)^{-1}S$ is nonnegative. Let $A(U)^{-1} = [\alpha_{ij}]$. Suppose that the main diagonal entries of S are $s_1, s_2, \dots, s_n$, then the ij-th entry of $SA(U)^{-1}S$ is $s_i \alpha_{ij} s_j$.

Without loss of generality, let us assume that 1 is a pendant vertex in U. Then, for any vertex i in U, there are at most two paths P_1 and P_2 (say) between 1 and i. As d is odd, the numbers of non-matching edges

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in both P_1 and P_2 are of the same parity. Let us take $s_i = (-1)^{n_i}$, where n_i is the number of non-matching edges in a path between 1 and i.

Suppose that the length of the cycle Γ is $2r+1$. From Theorem 2.7, it is clear that if there exists some i such that $\alpha_{ii} = \pm 2$, then U has exactly one peg and $r = d$. Moreover, if $\alpha_{ii} = \pm 2$, then $\alpha_{ii} = \frac{\det(U-i)}{\det(U)}$, where $\det(U-i) = (-1)^{m-r-1}2$ and $\det(U) = (-1)^m$. Therefore, $\alpha_{ii} = (-1)^{r-1}2 = (-1)^{d-1}2 = 2$, and it follows that the diagonal entries of $SA(U)^{-1}S$ are nonnegative.

Suppose that $\alpha_{ij} \neq 0$ such that $i \neq j$. Then a unique path exists between i and j, say P, such that $U - P$ has a unique spanning elementary subgraph H. Let k be a vertex on P with the minimum distance from the vertex 1. While calculating n_i, n_j, and n_k, it is important to consider the path that contains the vertex k. If $\alpha_{ij} = \pm 1$, then P is an mm-alternating path. Thus, $n_i + n_j - 2n_k = \frac{||P||-1}{2}$, where $||P||$ is the length of the path P. Note that H contains independent edges only as components and $|E(H)| = m - \frac{||P||+1}{2}$. Thus, by using Theorem 2.6, $\alpha_{ij} = (-1)^{m-\frac{||P||+1}{2}+||P||+m} = (-1)^{\frac{||P||-1}{2}}$. Therefore, $s_i\alpha_{ij}s_j = (-1)^{n_i+n_j+\frac{||P||-1}{2}} = 1$. Furthermore, if $\alpha_{ij} = \pm 2$, then H must contain Γ as one component. Notice that the number of non-matching edges in P is $\frac{||P||}{2}$ and hence, $n_i + n_j - 2n_k = \frac{||P||}{2}$. It is easy to observe that $|E(H)| = m + r - \frac{||P||}{2}$. By Theorem 2.7, U must have exactly one peg and hence $r = d$. Therefore, $\alpha_{ij} = (-1)^{r+1+\frac{||P||}{2}} \times 2$ and $s_i\alpha_{ij}s_j = (-1)^{n_i+n_j+r+1+\frac{||P||}{2}} \times 2 = (-1)^{r+1} \times 2 = 2$, as $r = d$ is odd. It follows that the matrix $SA(U)^{-1}S$ is nonnegative.

(ii) Suppose that d is even and 1 is a pendant vertex in U. Since d is an even number, for any vertex i in U, the number of matching edges in any two paths connecting the vertices 1 and i are of the same parity. Let us take the signature matrix S such that the i-th diagonal entry of S is $(-1)^{n_i}$, where n_i is the number of matching edges in a path between the vertices 1 and i. Using a similar approach as in part (i), it can be proved that $SA(U)^{-1}S$ is nonpositive. ∎

Below we provide an example to illustrate Theorem 3.1.

Example 3.2. Let U_1' and U_2' be graphs obtained by adding a pendant vertex to a vertex of the cycles C_3 and C_5, respectively, as shown in Fig. 3. Notice that $U_1', U_2' \in \mathcal{U}$ and U_1' has one matching edge in its unique cycle and U_2' has two matching edges in its unique cycle.

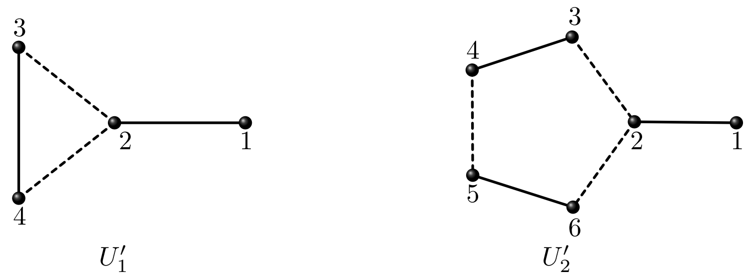

Figure 3. *Positively (left figure) and negatively (right figure) invertible non-bipartite unicyclic graphs with a unique perfect matching.*

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Consider the graph U_1'. Following Theorem 3.1 (i), observe that $s_1 = s_2 = 1$, $s_3 = s_4 = -1$, and

$$A(U_1')^{-1} = \begin{bmatrix} 2 & 1 & -1 & -1 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \end{bmatrix}.$$

Considering the signature matrix $S_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$, it is easy to check that the matrix

$$S_1A(U_1')^{-1}S_1 = \begin{bmatrix} 2 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix},$$

which is nonnegative. Thus, U_1' is positively invertible.

Similarly, taking $S_2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$, it can be verified that the matrix $S_2A(U_2')^{-1}S_2$ is nonpositive. Hence, the graph U_2' is negatively invertible.

The following is the main result of this section that presents the non-bipartite unicyclic graph with the minimum τ among all graphs in $\mathcal{U}_{2m}$.

THEOREM 3.3. *Let $m \geq 2$ and $\tilde{U}_{2m}$ be the unicyclic graph obtained from $P_{2m} = [1, 2, \ldots, 2m]$ by adding an edge between the vertices 1 and 3. Then*

$$\tau(U) \geq \tau(\tilde{U}_{2m}) \text{ for all } U \in \mathcal{U}_{2m},$$

and the equality holds if and only if U is isomorphic to $\tilde{U}_{2m}$.

Proof. Let $U \in \mathcal{U}_{2m}$ and e be a non-matching edge that lies in the unique cycle of U. Assume that $U - e$ is the graph obtained from U by deleting the edge e. Then, $U - e$ is a tree with a unique perfect matching. Thus, after a suitable ordering of the vertices of U, the adjacency matrix can be written in the following form:

$$A(U) = \begin{bmatrix} X & B \\ B^t & O \end{bmatrix},$$

where B is a lower triangular matrix with all its diagonal entries equal to 1 and $X = E_{ij} + E_{ji}$, for $1 \leq i < j \leq m$. Then, the adjacency matrix of the graph U^+ is

$$A(U)^{-1} = \begin{bmatrix} O & (B^{-1})^t \\ B^{-1} & Y \end{bmatrix}, \text{ where } Y = -B^{-1}X(B^{-1})^t.$$

Let us relabel the vertices of $\tilde{U}_{2m}$ as described in Fig. 4.

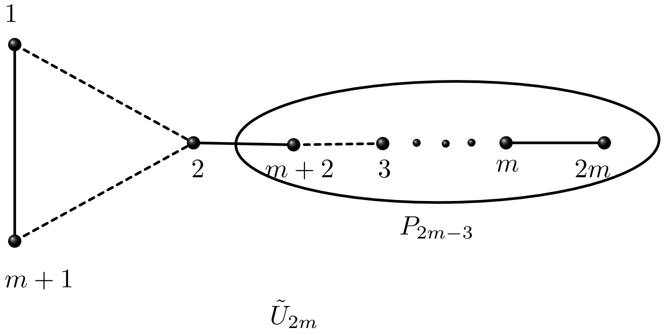

FIGURE 4. *Non-bipartite unicyclic graph $\tilde{U}_{2m}$ with a unique perfect matching having the minimum τ.*

Then, the adjacency matrix of $\tilde{U}_{2m}$ can be expressed as:

$$A(\tilde{U}_{2m}) = \begin{bmatrix} \tilde{X} & \tilde{B} \\ \tilde{B}^t & O \end{bmatrix},$$

where $\tilde{B} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 1 \end{bmatrix}$ and $\tilde{X} = E_{12}+E_{21}$. By using Theorem 3.1, $\tilde{U}_{2m}$ is positively invertible. So $A(\mathbf{\tilde{U}^+_{2m}})$ and $A(\tilde{U}_{2m})^{-1}$ are diagonally similar. Observe that

$$A(\mathbf{\tilde{U}^+_{2m}}) = \begin{bmatrix} O & (|\tilde{B}^{-1}|)^t \\ |\tilde{B}^{-1}| & \tilde{Y} \end{bmatrix},$$

where $|\tilde{B}^{-1}| = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & \cdots & 0 \\ 1 & 1 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{bmatrix}$ and $\tilde{Y} = |-\tilde{B}^{-1}\tilde{X}(\tilde{B}^{-1})^t| = \begin{bmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 2 & 2 & \cdots & 2 \\ 1 & 2 & 2 & \cdots & 2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 2 & 2 & \cdots & 2 \end{bmatrix}$.

Now, we prove that $|A(U)^{-1}| \leq A(\mathbf{\tilde{U}^+_{2m}})$. It is easy to verify that $|B^{-1}| \leq |\tilde{B}^{-1}|$. Further, notice that the entries of Y are from the set $\{0, 1, -1, 2, -2\}$ and the edge e connects the vertices i and j, where $1 \leq i < j \leq m$. Then, we have the following two cases.

Case I. Let $i > 1$. Note that the matching edges of U are $\{1, m+1\}, \dots, \{m, 2m\}$. The vertex $m+1$ is a quasi-pendant vertex in U and thus, by using Theorem 2.6, each entry of the first row and first column of Y is 0. Hence, $|Y| \leq \tilde{Y}$.

Case II. Let $i = 1$. Then the vertex $m+1$ is in the unique cycle of U. Thus, $U - \{m+1\}$ is a singular tree. Hence, the $(m+1)$-th diagonal entry of $A(U)^{-1}$, which is same as the $(1,1)$-th entry of Y, is 0. Again by applying Theorem 2.6, the other entries of the first row and first column of Y cannot be ± 2. Hence, $|Y| \leq \tilde{Y}$.

Thus, in both the cases $|A(U)^{-1}| \leq A(\mathbf{\tilde{U}^{+}_{2m}})$. Hence, by using Theorem 2.2, $\rho(U^{+}) \leq \rho(\mathbf{\tilde{U}^{+}_{2m}})$. Note that $\rho(\mathbf{\tilde{U}^{+}_{2m}}) = \frac{1}{\tau(\tilde{U}_{2m})}$ and $\rho(U^{+}) \geq \lambda_{2m}(U^{+}) = \frac{1}{\tau(U)}$. Therefore, $\frac{1}{\tau(U)} \leq \frac{1}{\tau(\tilde{U}_{2m})}$, which implies that $\tau(\tilde{U}_{2m}) \leq \tau(U)$.

Further, if $\tau(U) = \tau(\tilde{U}_{2m})$, then $\rho(\mathbf{\tilde{U}^{+}_{2m}}) = \lambda_{2m}(U^{+}) = \rho(U^{+})$ as $\rho(U^{+}) \leq \rho(\mathbf{\tilde{U}^{+}_{2m}})$. The condition $\lambda_{2m}(U^{+}) = \rho(U^{+})$ implies that U is positively invertible. Therefore, by Theorem 2.3, we can conclude that there exists a signature matrix S such that $A(\mathbf{\tilde{U}^{+}_{2m}}) = SA(U)^{-1}S$, which implies that U is isomorphic to $\tilde{U}_{2m}$. ∎

Remark 3.4. Note that $\tau(\tilde{U}_n)$ decreases as n increases and $\lim_{n\to\infty} \tau(\tilde{U}_n) = 0$. Thus, the graph in $\mathcal{U}$ with the minimum τ cannot be obtained.

4. Non-bipartite unicyclic graphs with a unique perfect matching having maximum τ. In this section, we characterize the graphs U having maximum τ among all the graphs in $\mathcal{U}_n$. Prior to that, we prove the following important result relating the smallest positive eigenvalues of a nonsingular graph G and its induced nonsingular subgraph H.

Lemma 4.1. *Let G be a nonsingular graph on $n \geq 4$ vertices with an induced nonsingular subgraph H such that $H' = G - H$ is bipartite and nonsingular. Let $V(H') = X \cup Y$ be the bipartition of the vertex set of H'. If the vertices in the set Y are not adjacent to any vertex of H in the graph G, then H^{+} is an induced subgraph of G^{+}. Moreover, $\tau(G) \leq \tau(H)$.*

Proof. Suppose that $A(H') = \begin{bmatrix} O & B \\ B^t & O \end{bmatrix}$ is the adjacency matrix of the graph H'. Then, the adjacency matrix of the graph G can be written as

$$A(G) = \begin{bmatrix} A(H) & C & O \\ C^t & O & B \\ O^t & B^t & O \end{bmatrix},$$

where C represents the adjacency between the vertices in H and X. Then, the Schur complement of the block matrix $A(H')$ is

$$\begin{aligned} M_{A(H')} &= A(H) - \begin{bmatrix} C & O \end{bmatrix} A(H')^{-1} \begin{bmatrix} C^t \\ O^t \end{bmatrix} \\ &= A(H) - \begin{bmatrix} C & O \end{bmatrix} \begin{bmatrix} O & (B^{-1})^t \\ B^{-1} & O \end{bmatrix} \begin{bmatrix} C^t \\ O^t \end{bmatrix} \\ &= A(H). \end{aligned}$$

Now, using Lemma 2.4, $A(H)^{-1}$ is a principal submatrix of $A(G)^{-1}$. Thus, H^{+} is an induced subgraph of G^{+}. As a result, we have $\lambda_n(H^{+}) \leq \lambda_n(G^{+})$ and hence, $\tau(G) \leq \tau(H)$. ∎

Remark 4.2. Since the position of τ is not fixed in the spectrum of an arbitrary graph, we could not prove Lemma 4.1 by applying the interlacing theorem (Theorem 2.1) directly.

Let U be a unicyclic graph with a unique perfect matching. From the Rational Root Theorem, we know that $\frac{1}{2}$ cannot be an eigenvalue of $A(U)$. The following result from [5] reveals that except two graphs, all other bipartite unicyclic graphs with a unique perfect matching have smallest positive eigenvalue less than $\frac{1}{2}$.

THEOREM 4.3. (Barik and Behera [5]) *Let U be a bipartite unicyclic graph with a unique perfect matching. Then, $\tau(U) < \frac{1}{2}$ if and only if U is not isomorphic to the graph G_1 or G_2 as depicted in Fig. 5.*

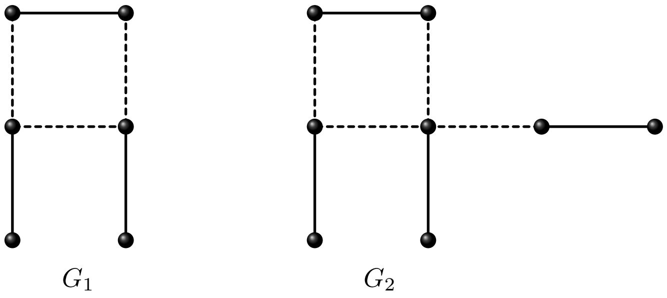

FIGURE 5. *Bipartite unicyclic graphs with $\tau > \frac{1}{2}$.*

Note that $\tau(G_1) \approx 0.5550 > \frac{1}{2}$ and $\tau(G_2) \approx 0.5028 > \frac{1}{2}$. This establishes that among all bipartite unicyclic graphs with a unique perfect matching, G_1 is the unique graph with the largest τ and G_2 is the unique graph with the second largest τ. We look forward characterizing the graphs having maximum τ among all the non-bipartite unicyclic graphs with a unique perfect matching.

Let us define the following class of non-bipartite unicyclic graphs with girth 5.

DEFINITION 4.4. Let $\mathcal{U}^*$ be the class of all graphs in $\mathcal{U}$ with $g(U) = 5$ and $p(U) = 1$ such that if Γ is the unique cycle in U and $\{u, v\}$ is the peg in U, then except the vertex v, the other four vertices in Γ have degree exactly 2.

EXAMPLE 4.5. The graphs U_1 and U_2 drawn in Fig. 6 are constructed using Definition 4.4. Hence, $U_1, U_2 \in \mathcal{U}^*$. Note that $\tau(U_1) \approx 0.5015 > \frac{1}{2}$ and $\tau(U_2) \approx 0.4825 < \frac{1}{2}$.

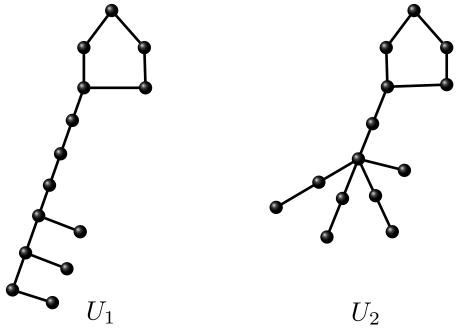

FIGURE 6. *Graphs U_1 and U_2 in $\mathcal{U}^*$ with $\tau(U_1) \approx 0.5015 > \frac{1}{2}$ and $\tau(U_2) \approx 0.4825 < \frac{1}{2}$.*

Our next result characterizes all the non-bipartite unicyclic graphs with a unique perfect matching that are in $\mathcal{U} \setminus \mathcal{U}^*$ having $\tau > \frac{1}{2}$. Interestingly, there are exactly three such graphs.

THEOREM 4.6. *Let $U \in \mathcal{U} \setminus \mathcal{U}^*$. Then, $\tau(U) > \frac{1}{2}$ if and only if U is isomorphic to H_1, H_2, H_3 drawn in Fig. 7.*

Proof. Suppose that U is of order $2m$, $m \geq 2$. Note that $p(U)$ is always odd. Let us first consider the case when $p(U) > 1$.

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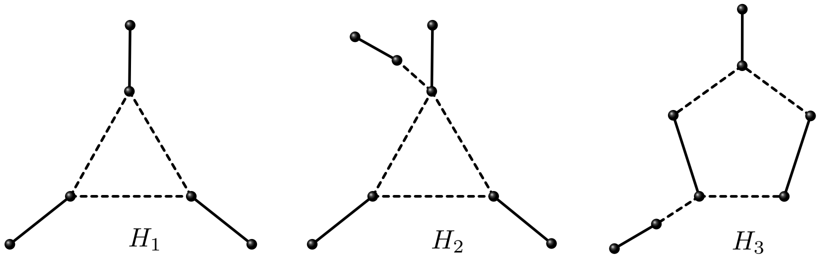

FIGURE 7. *Non-bipartite unicyclic graphs* H_1*,* H_2*, and* H_3 *with a unique perfect matching having* $\tau > \frac{1}{2}$*;* $\tau(H_1) = \frac{\sqrt{5}-1}{2}, \tau(H_2) \approx 0.5038$ *and* $\tau(H_3) \approx 0.5013$*.*

Now, if $g(U) > p(U)$, then observe that there exist two pegs $\{u, v\}, \{u', v'\}$ in U such that the mm-alternating path between the vertices u and u' has length at least 5. Let $P = [u, v, v_1, v_2, \ldots, v_l, v', u']$ be an alternating path between the vertices u and u', see Fig. 8.

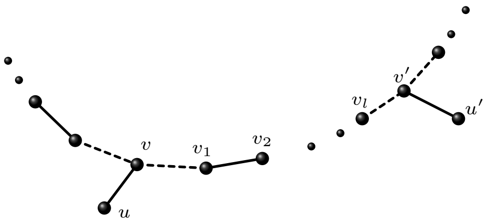

FIGURE 8. *The graph* $U \in \mathcal{U}_{2m}$ *with* $p(U) > 1$ *and* $g(U) > p(U)$*.*

Note that P is an induced nonsingular subgraph of U such that $U - P$ is a nonsingular forest. Since $g(U)$ is odd, P satisfies all the conditions of Lemma 4.1. Thus, we have $\tau(U) \leq \tau(P) < \frac{1}{2}$, as P is the path with at least six vertices.

If $g(U) = p(U)$, then U must contain $\hat{C}_g$ as an induced subgraph, where $g = g(U)$. Thus, by Lemma 4.1, $\tau(U) \leq \tau(\hat{C}_g)$. Since g is odd, the smallest eigenvalue of C_g is $-2\cos\frac{\pi}{g}$. By applying Theorem 2.8, we get that, if $g \geq 5$, then the smallest eigenvalue of $\hat{C}_g$ is less than -2, which implies that $\tau(U) < \frac{1}{2}$.

If $g = 3$, then $\tau(\hat{C}_3) = \frac{\sqrt{5}-1}{2} > \frac{1}{2}$. In this case, if $m = 3$, then U is the graph H_1 in Fig. 7. If $m \geq 4$, then U contains either H_2 (see Fig. 7) or H_2' (see Fig. 9) as a nonsingular induced subgraph. By direct computation, it can be verified that $\tau(H_2') < \frac{1}{2}$. Thus, if U contains H_2' as an induced subgraph, then $\tau(U) \leq \tau(H_2') < \frac{1}{2}$.

Suppose that U contains H_2 as an induced subgraph. Now, if $m = 4$ then $U = H_2$ and $\tau(U) > \frac{1}{2}$. If $m \geq 5$, then U must contain one of the graphs U_1, U_2, U_3, and U_4 (see Fig. 9) as an induced subgraph. It is easy to verify that $\tau(U_i) < \frac{1}{2}$ for $i = 1, \ldots, 4$. This implies that $\tau(U) < \frac{1}{2}$.

Now, consider the case $p(U) = 1$. Let Γ be the unique cycle in U. If $g(U) \geq 7$, then U has an alternating path P_1 of length 5 that lies in Γ such that $U - P_1$ is a nonsingular forest. Then by Lemma 4.1, $\tau(U) \leq \tau(P_1) < \frac{1}{2}$.

If $g(U) = 3$, then the graph H (Fig. 10) is an induced subgraph of U. Since $\tau(H) < \frac{1}{2}$, by using Lemma 4.1, $\tau(U) \leq \tau(H) < \frac{1}{2}$.

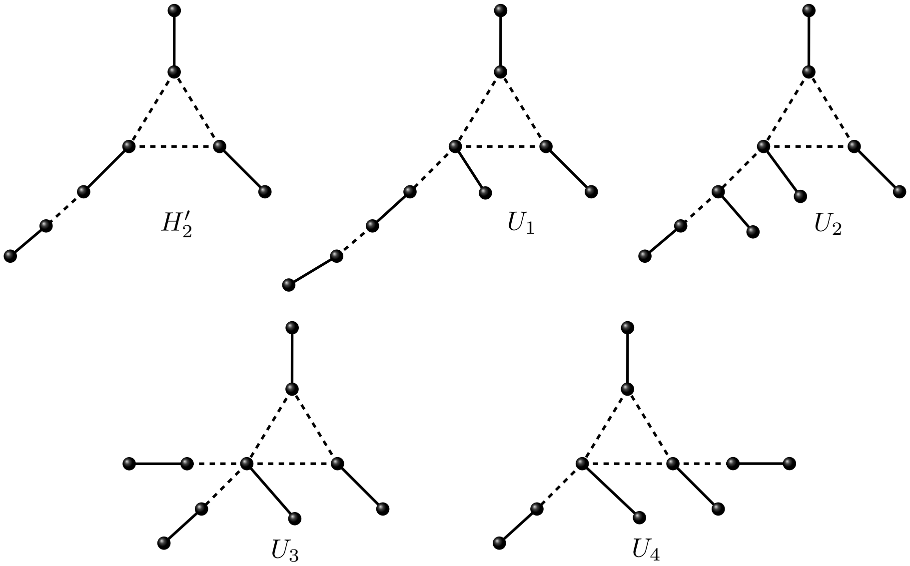

FIGURE 9. *Some graphs in $\mathcal{U}_8$ and $\mathcal{U}_{10}$ with girth 3 and exactly three pegs.*

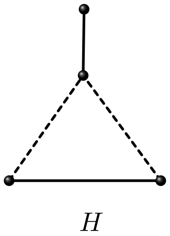

FIGURE 10. *The unique non-bipartite graph with a unique perfect matching on four vertices; $\tau(H) \approx 0.3111$.*

Finally, if $g(U) = 5$, then $m \geq 4$ and there are at least two vertices of degree greater than or equal to 3 in Γ (as $U \notin \mathcal{U}^*$). Now, if $m = 4$, then by direct computation, we can conclude that the only graph with $\tau > \frac{1}{2}$ is H_3, which is drawn in the Fig. 7.

If $m = 5$, then we have 14 such graphs as drawn in Fig. 11: 10 with two vertices of the cycle with degree at least 3; 4 with three vertices of the cycle with degree at least 3 (G_3, G_5, G_6, and G_{10}). By direct computation, it can be checked easily that $\tau(G_i) < \frac{1}{2}$, for $i = 1, \ldots, 14$.

If $m \geq 6$, then observe that U is obtained by adding an even number of edges to some G_i, $i = 1, \ldots, 14$. In other words, G_i for some $i = 1, \ldots, 14$ is an induced subgraph of U. Thus, by Lemma 4.1, $\tau(U) \leq \tau(G_i)$ for some $i = 1, \ldots, 14$. Since $\tau(G_i) < \frac{1}{2}$ for all $i = 1, \ldots, 14$, the proof follows. ∎

The following result gives an upper bound on the smallest positive eigenvalue of the graphs that are in $\mathcal{U}$.

THEOREM 4.7. *Let U be a non-bipartite unicyclic graph with a unique perfect matching. Then $\tau(U) \leq \frac{\sqrt{5}-1}{2}$.*

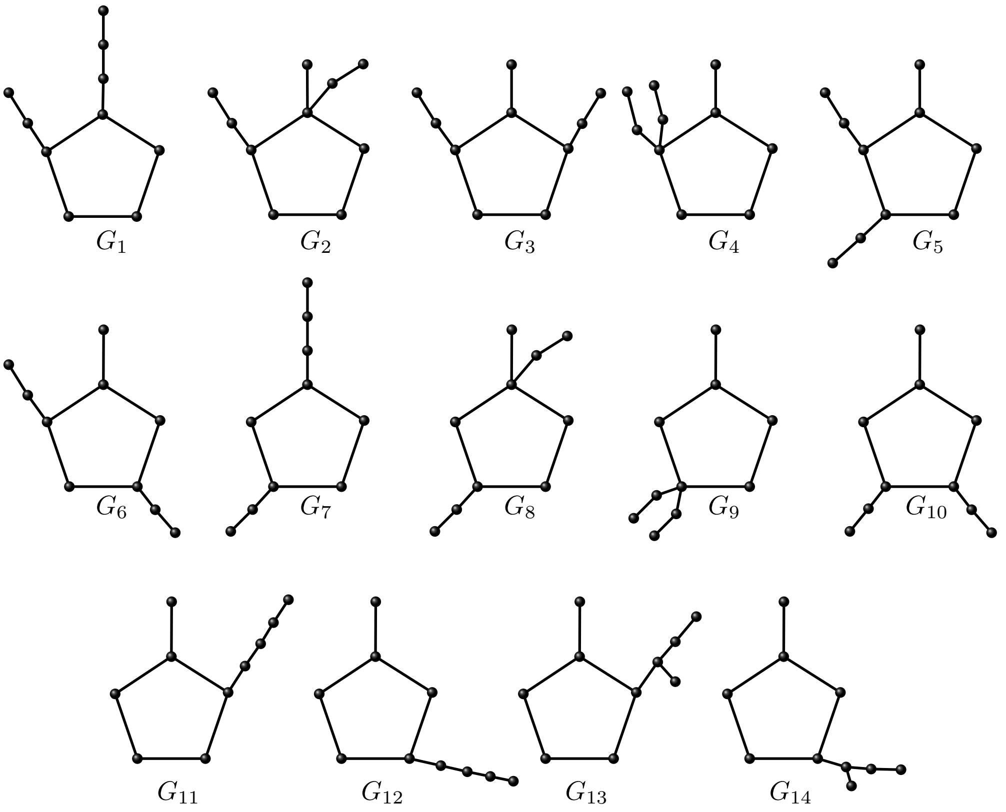

FIGURE 11. *Non-bipartite unicyclic graphs on* 10 *vertices with a unique perfect matching having exactly one peg and girth* 5 *such that the degree of at least two vertices in* Γ *are greater than* 2.

Proof. If $U \in \mathcal{U} \setminus \mathcal{U}^*$, then by Theorem 4.6, $\tau(U) > \frac{1}{2}$ if and only if U is isomorphic to the graph H_1, H_2, H_3 illustrated in Fig. 7. Furthermore, $\tau(H_2) < \frac{\sqrt{5}-1}{2}$, $\tau(H_3) < \frac{\sqrt{5}-1}{2}$, and $\tau(H_1) = \frac{\sqrt{5}-1}{2}$. Therefore, if $U \notin \mathcal{U}^*$, then $\tau(U) \leq \frac{\sqrt{5}-1}{2}$. Moreover, H_1 is the unique graph in $\mathcal{U} \setminus \mathcal{U}^*$ having $\tau = \frac{\sqrt{5}-1}{2}$.

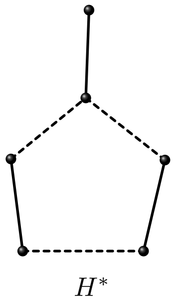

FIGURE 12. *The unique graph* $H^* \in \mathcal{U}^*$ *of order* 6.

Now, if $U \in \mathcal{U}^*$, then U contains the graph H^* (see Fig. 12) as an induced subgraph. Then by Lemma 4.1, we have $\tau(U) \leq \tau(H^*) = \frac{\sqrt{5}-1}{2}$. ∎

Now, we proceed for a characterization of graphs in $\mathcal{U}_n$ having maximum τ. Let us define the following subclass of graphs of $\mathcal{U}^*$.

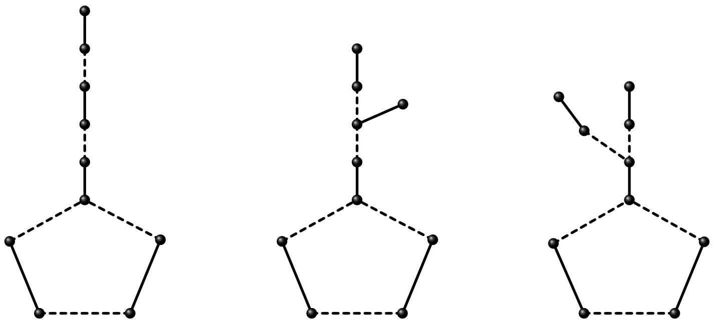

FIGURE 13. *All possible graphs in* $\mathcal{U}_{10}^{**}$.

DEFINITION 4.8. Let $T_1, \ldots, T_k$ be k trees such that $T_i = P_2$ or P_4 for each $i = 1, \ldots, k$. Take a copy of H^* and name the pendant vertex of H^* as u. Identify k vertices $x_1, \ldots, x_k$, where x_i is a vertex of T_i. Let G be the graph obtained by joining the vertices $x_1, \ldots, x_k$ of the trees $T_1, \ldots, T_k$ with the vertex u of the graph H^*. Let $\mathcal{U}_n^{**}$ be the collection of such graphs G with $n = 2m$ vertices, for $m \geq 4$. See for example the graphs drawn in Fig. 13 that are in $\mathcal{U}_{10}^{**}$.

One of the significant findings of this section, which characterizes the graphs with maximum τ in $\mathcal{U}_n$, is given below.

THEOREM 4.9. *Let* $m \geq 3$ *and* U *be a non-bipartite unicyclic graph with a unique perfect matching on* $n = 2m$ *vertices. Then* $\tau(U) \leq \frac{\sqrt{5}-1}{2}$. *Further,*

(i) *if* $n = 6$, *then the equality holds if and only if either* U *is isomorphic to* $H_1 = \hat{C_3}$ *or* H^* *(see Fig. 12);*
(ii) *If* $n \geq 8$, *the equality holds if and only if* U *is isomorphic to* H^{**} *(see Fig. 14) or* $U \in \mathcal{U}_n^{**}$.

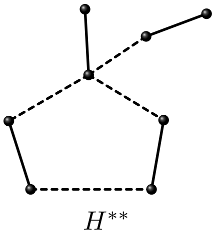

FIGURE 14. *The graph* H^{**}.

Proof. Note that if $U \in \mathcal{U} \setminus \mathcal{U}^*$, then by the argument of the proof of Theorem 4.7, $\tau(U) = \frac{\sqrt{5}-1}{2}$ if and only if U is isomorphic to $\hat{C_3}$.

Let $U \in \mathcal{U}^*$ and Γ be the unique cycle in U. Then by Theorem 4.7, $\tau(U) \leq \frac{\sqrt{5}-1}{2}$. We now characterize the graphs in $\mathcal{U}^*$ with $\tau = \frac{\sqrt{5}-1}{2}$. Note that $n \geq 6$. Now, if $n = 6$, then U is the graph H^* as drawn in Fig. 12, and $\tau(U) = \frac{\sqrt{5}-1}{2}$.

If $n \geq 8$, then U has a unique structure as drawn in Fig. 15, which is obtained from H^*. Let $\{u, v\}$ be the peg in H^* such that $v \in \Gamma$. Let $T_1, \ldots, T_r, T'_1, \ldots, T'_s$ be nonsingular trees such that some vertex of each T_i is adjacent with u and some vertex of each T'_j is adjacent with v, respectively (see Fig. 15).

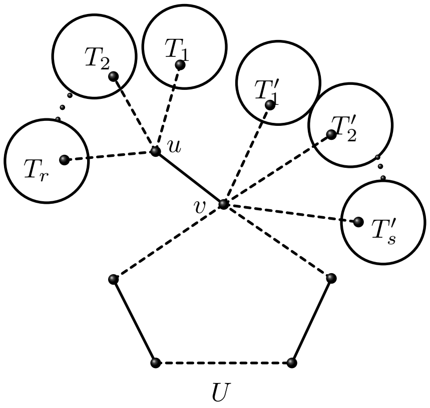

FIGURE 15. *Structure of graphs $U \in \mathcal{U}^*$.*

We have the following cases:

Case 1. If $s \geq 2$, then H_1^* (refer Fig. 16) is an induced subgraph of U such that $U - H_1^*$ is nonsingular forest. Thus, by Lemma 4.1, $\tau(U) \leq \tau(H_1^*) < \frac{\sqrt{5}-1}{2}$.

Case 2. Let $s = 1$. Consider the graphs H_2^*, H_3^*, and H_4^* in Fig. 16. Now, if $V(T_1') \geq 4$, then in a similar approach we can show that either $\tau(U) \leq \tau(H_2^*) < \frac{\sqrt{5}-1}{2}$ or $\tau(U) \leq \tau(H_3^*) < \frac{\sqrt{5}-1}{2}$.

If $V(T_1') = 2$, that is, $T_1' = P_2$, then we have $\tau(U) \leq \tau(H_4^*) < \frac{\sqrt{5}-1}{2}$ unless $r = 0$. Further, if $r = 0$, then $U = H^{**}$ (see Fig. 14) and hence $\tau(U) = \frac{\sqrt{5}-1}{2}$.

Case 3. Let $s = 0$. If there exists at least one tree branch, say T_1, such that $|V(T_1)| \geq 6$, then $\tau(U) \leq \tau(H_i^*) < \frac{\sqrt{5}-1}{2}$ (using τ values from Table 1), for some $i = 5, \ldots, 11$, where the graph H_i^* is illustrated in Fig. 16. If $|V(T_i)| \leq 4$ for all $i = 1, \ldots, r$, then $U \in \mathcal{U}_n^{**}$.

TABLE 1
The approximate values of τ for each graph defined in Fig. 16.

G	H_1^*	H_2^*	H_3^*	H_4^*	H_5^*	H_6^*	H_7^*	H_8^*	H_9^*	H_{10}^*	H_{11}^*
$\tau(G)$	0.5862	0.4833	0.5473	0.5678	0.5115	0.4621	0.4936	0.5276	0.5482	0.5669	0.5370

Next, we show that $\tau(U) = \frac{\sqrt{5}-1}{2}$ if $U \in \mathcal{U}_n^{**}$. Consider the graph $U - u = \Gamma \cup T_1 \cup \cdots \cup T_r$. Note that $A(U-u)$ is a principal minor of $A(U)$ and the number of positive eigenvalues of U and $U - u$ are the same. Thus, by using Theorem 2.1, we have $\tau(U) \geq \tau(U-u) = \min\{\tau(\Gamma), \tau(T_1), \ldots, \tau(T_r)\} = \frac{\sqrt{5}-1}{2}$ as each $T_i = P_2$ or P_4.

Thus, for the case $n \geq 8$, if $U \in \mathcal{U}^*$ and $\tau(U) = \frac{\sqrt{5}-1}{2}$, then either U is isomorphic to H^{**} (see Fig. 14) or $U \in \mathcal{U}_n^{**}$. This completes the proof. ∎

REMARK 4.10. Notice that all the graphs $U \in \mathcal{U}$ with $\tau(U) = \frac{\sqrt{5}-1}{2}$ are negatively invertible.

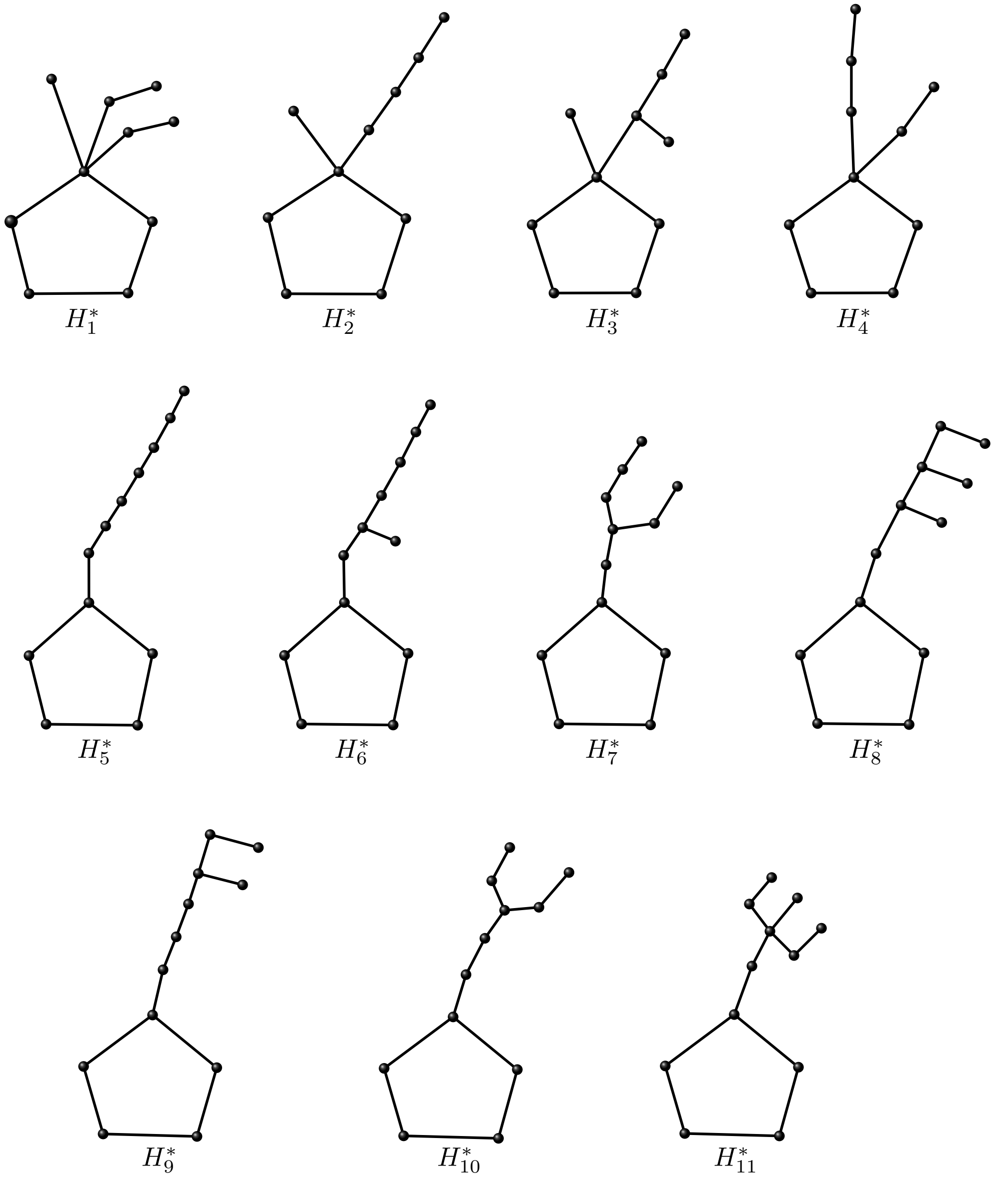

FIGURE 16. *Some graphs in* $\mathcal{U}^*$ *with* $\tau < \frac{\sqrt{5}-1}{2}$.

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Declaration of competing interest.

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Data availability.

No data was used for the research described in the article.

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