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Resolvent Energy of Unicyclic, Bicyclic and Tricyclic Graphs

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Abstract

The resolvent energy of a graph G of order n is defined as $ER = \sum_{i=1}^{n}(n-\lambda_i)^{-1}$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of G. In a recent work [Gutman et al., *MATCH Commun. Math. Comput. Chem.* **75** (2016) 279–290] the structure of the graphs extremal w.r.t. ER were conjectured, based on an extensive computer–aided search. We now confirm the validity of some of these conjectures.

1 Introduction

Let G be a graph on n vertices, and let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be its eigenvalues, that is, the eigenvalues of the adjacency matrix of G. The resolvent energy of G is defined in [3,4] as

$$ER(G) = \sum_{i=1}^{n} \frac{1}{n-\lambda_i} \,. \tag{1}$$

It was shown in [3] that

$$ER(G) = \frac{1}{n} \sum_{k=0}^{\infty} \frac{M_k(G)}{n^k} \tag{2}$$

where $M_k(G) = \sum_{i=1}^{n} \lambda_i^k$ is the k-th spectral moment of G.

In what follows, we present results found in the literature that confirm some of the conjectures made in [3, 4] on the resolvent energy of unicyclic, bicyclic and tricyclic graphs. These results were originally stated in [2,5,6] in terms of the Estrada index, another spectrum–based graph invariant related to the spectral moments by the formula

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!} \, .$$

Most of the proofs in [2, 5, 6] are based on the spectral moments and work for the resolvent energy without any change. The proofs that involve direct calculations with Estrada indices can be easily modified to give the equivalent results concerning the resolvent energy, as we show below. Thus, the following are determined:

- the unicyclic graph with maximum resolvent energy (Theorem 1);
- the unicyclic graphs with minimum resolvent energy (Theorems 2 and 3);
- the bicyclic graph with maximum resolvent energy (Theorem 4);
- the tricyclic graph with maximum resolvent energy (Theorem 5).

2 Unicyclic graphs with maximum and minimum resolvent energy

Let X_n denote the unicyclic graph obtained from the cycle C_3 by attaching $n - 3$ pendent vertices to one of its vertices, and $\tilde{X}_n$ the unicyclic graph obtained from C_4 by attaching $n - 4$ pendent vertices to one of its vertices, as in Figure 1.

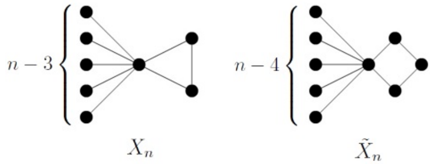

Figure 1: Unicyclic graphs with maximum resolvent energy.

Lemma 1. *Let G be a unicyclic graph on $n \geq 4$ vertices, $G \ncong X_n, \tilde{X}_n$.*

1. *If G is bipartite, then $M_k(G) \leq M_k(\tilde{X}_n)$, for all $k \geq 0$, and $M_{k_0}(G) < M_{k_0}(\tilde{X}_n)$ for some k_0.*

2. *If G is not bipartite (that is, G contains an odd cycle), then $M_k(G) \leq M_k(X_n)$ for all $k \geq 0$, and $M_{k_0}(G) < M_{k_0}(X_n)$ for some k_0.*

Proof. Part (i) follows from Lemmas 3.2, 3.5 and 3.8 in [2], and (ii) follows from Lemmas 3.2, 3.5 and 3.7 in [2]. □

We denote the characteristic polynomial of a graph G by $\phi(G,\lambda)$. For a proper subset V_1 of $V(G)$, $G - V_1$ denotes the graph obtained from G by deleting the vertices in V_1 (and the edges incident on them). Let $G - v = G - \{v\}$, for $v \in V(G)$. We make use of the following lemma.

Lemma 2. [1] *Let $v \in V(G)$, and let $\mathcal{C}(v)$ be the set of cycles containing v. Then*

$$\phi(G,\lambda) = \lambda\,\phi(G-v,\lambda) - \sum_{vw \in E(G)} \phi(G-v-w,\lambda) - 2\sum_{Z \in \mathcal{C}(v)} \phi(G-V(Z),\lambda)$$

where $\phi(G-v-w,\lambda) \equiv 1$ if G is a single edge, and $\phi(G-VZ,\lambda) \equiv 1$ if G is a cycle.

Theorem 1. *Let G be a unicyclic graph on $n \geq 4$ vertices. Then $ER(G) \leq ER(X_n)$, with equality if and only if $G \cong X_n$. Moreover, if G is bipartite, then $ER(G) \leq ER(\tilde{X}_n)$, with equality if and only if $G \cong \tilde{X}_n$.*

Proof. Let G be a unicyclic graph. Lemma 1 and equation (2) imply that $ER(G) \leq ER(X_n)$ if G contains an odd cycle, and $ER(G) \leq ER(\tilde{X}_n)$ if G contains an even cycle (i.e., G is bipartite). Furthermore, equality occurs if and only if $G \cong X_n$, in the case of an odd cycle, or $G \cong \tilde{X}_n$, in the bipartite case.

Now, an n-vertex unicyclic graph with maximum resolvent energy is either X_n or $\tilde{X}_n$. We show that $ER(X_n) > ER(\tilde{X}_n)$, for $n \geq 4$. Let $\phi(X_n, \lambda)$ and $\phi(\tilde{X}_n, \lambda)$ denote the characteristic polynomials of X_n and $\tilde{X}_n$, respectively. Then, by [3, Theorem 8], we have

$$ER(X_n) = \frac{\phi'(X_n, n)}{\phi(X_n, n)} \qquad \text{and} \qquad ER(\tilde{X}_n) = \frac{\phi'(\tilde{X}_n, n)}{\phi(\tilde{X}_n, n)} \tag{3}$$

where $\phi'(G, \lambda) = \frac{d}{d\lambda}\,\phi(G, \lambda)$. By Lemma 2, it follows that

$$\begin{aligned}
\phi(X_n, \lambda) &= \lambda^{n-4}\,(\lambda^4 - n\lambda^2 - 2\lambda + n - 3) \\
\phi(\tilde{X}_n, \lambda) &= \lambda^{n-4}\,(\lambda^4 - n\lambda^2 + 2n - 8)\,.
\end{aligned}$$

Hence

$$\begin{aligned}
ER(X_n) - ER(\tilde{X}_n) &= \frac{\phi'(X_n, n)}{\phi(X_n, n)} - \frac{\phi'(\tilde{X}_n, n)}{\phi(\tilde{X}_n, n)} \\
&= \frac{\phi'(X_n, n)\,\phi(\tilde{X}_n, n) - \phi'(\tilde{X}_n, n)\,\phi(X_n, n)}{\phi(X_n, n)\,\phi(\tilde{X}_n, n)} \\
&= \frac{10n^4 - 24n^3 + 10n^2 - 4n + 16}{(n^4 - n^3 - n - 3)(n^4 - n^3 + 2n - 8)}\,.
\end{aligned}$$

The polynomial $p(\lambda) = 10\lambda^4 - 24\lambda^3 + 10\lambda^2 - 4\lambda + 16$ does not have any real roots, thus the numerator $p(n)$ is positive for all n. The real roots of the polynomials $\lambda^4 - \lambda^3 - \lambda - 3$ and $\lambda^4 - \lambda^3 + 2\lambda - 8$ are less than 2, so the denominator is positive for $n \geq 2$. It follows that $ER(X_n) - ER(\tilde{X}_n) > 0$. $\square$

Let C_n^* denote the unicyclic graph obtained by attaching a pendent vertex to a vertex of C_{n-1}.

Lemma 3. *Let G be a unicyclic graph on $n \geq 5$ vertices. If $G \ncong C_n, C_n^*$, then at least one of the following holds:*

1. *$M_k(G) \geq M_k(C_n)$ for all $k \geq 0$, and $M_k(G) > M_k(C_n)$ for some $k_0 \geq 0$.*

2. $M_k(G) \geq M_k(C_n^*)$ *for all* $k \geq 0$*, and* $M_k(G) > M_k(C_n^*)$ *for some* $k_0 \geq 0$*.*

Proof. If $G \ncong C_n, C_n^*$, it follows from Lemmas 5.3, 5.4, 5.5 in [2] that G can be transformed into either C_n or C_n^* in a finite number of steps, in such a way that, at each step, the k-th spectral moment does not increase for each k, and decreases for some k_0. □

Theorem 2. *Let* G *be a unicyclic graph on* $n \geq 5$ *vertices. If* $G \ncong C_n, C_n^*$*, then* $ER(G) > \min\{ER(C_n), ER(C_n^*)\}$*.*

Proof. Follows from Lemma 3. □

Using arguments that are not based on spectral moments, we can strengthen Theorem 2 as follows:

Theorem 3. *Let* G *be a unicyclic graph on* $n \geq 5$ *vertices. If* $G \ncong C_n$*, then* $ER(G) > ER(C_n)$*.*

Proof. In view of Theorem 2, it is sufficient to prove that $ER(C_n) < ER(C_n^*)$. In [3], the validity of this latter inequality was checked for $n \leq 15$. Therefore, in what follows we may asume that $n > 15$, i.e., that n is sufficiently large.

Bearing in mind the relations (3), we get

$$ER(G) = \left.\frac{d \ln \phi(G,\lambda)}{d\lambda}\right|_{\lambda=n}$$

and therefore

$$\begin{aligned} ER(C_n) - ER(C_n^*) &= \left.\left(\frac{d \ln \phi(C_n,\lambda)}{d\lambda} - \frac{d\phi(\ln C_n^*,\lambda)}{d\lambda}\right)\right|_{\lambda=n} \\ &= \left.\frac{d}{d\lambda} \ln \frac{\phi(C_n,\lambda)}{\phi(C_n^*,\lambda)}\right|_{\lambda=n} . \end{aligned} \tag{4}$$

The greatest eigenvalue of C_n is 2, and the greatest eigenvalue of C_n^* is certainly less than 3. Therefore, bearing in mind that C_n and C_n^* contain no triangles and no pentagons, for $\lambda = n$,

$$\begin{aligned} \phi(C_n,\lambda) &= \lambda^n - n\,\lambda^{n-2} + b_2(C_n)\,\lambda^{n-4} + \cdots \\ \phi(C_n^*,\lambda) &= \lambda^n - n\,\lambda^{n-2} + b_2^*(C_n)\,\lambda^{n-4} + \cdots \end{aligned}$$

and thus

$$\frac{\phi(C_n,\lambda)}{\phi(C_n^*,\lambda)} = 1 + \frac{b_2(C_n) - b_2(C_n^*)}{\lambda^4} + O\left(\frac{1}{\lambda^6}\right)$$

and

$$\ln \frac{\phi(C_n,\lambda)}{\phi(C_n^*,\lambda)} = \frac{b_2(C_n) - b_2(C_n^*)}{\lambda^4} + O\left(\frac{1}{\lambda^6}\right).$$

Then because of (4),

$$ER(C_n) - ER(C_n^*) = -4\,\frac{b_2(C_n) - b_2(C_n^*)}{n^5} + O\left(\frac{1}{n^7}\right). \tag{5}$$

Using the Sachs coefficient theorem [1], one can easily show that

$$b_2(C_n) = \frac{1}{2}\,n(n-3) \qquad \text{and} \qquad b_2(C_n^*) = \frac{1}{2}\,(n-3)(n-4) + 2n - 7$$

from which one immediately gets that for sufficiently large values of n,

$$ER(C_n) - ER(C_n^*) \approx -\frac{4}{n^5}$$

i.e., $ER(C_n) < ER(C_n^*)$. □

3 Bicyclic graphs with maximum resolvent energy

Let $\theta(p,q,\ell)$ be the union of three internally disjoint paths $P_{p+1}, P_{q+1}, P_{\ell+1}$ with common end vertices. Let Y_n denote the bicyclic graph obtained from $\theta(2,2,1)$ by attaching $n-4$ pendent vertices to one of its vertices of degree 3, and let $\tilde{Y}_n$ denote the bicyclic graph obtained from $\theta(2,2,2)$ by attaching $n-5$ pendent vertices to one of its vertices od degree 3, as in Figure 2.

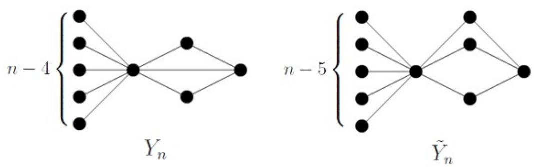

Figure 2: Bicyclic graphs with maximum resolvent energy.

Lemma 4. *Let G be a bicyclic graph on $n \geq 5$ vertices, $G \ncong Y_n, \tilde{Y}_n$. Then one of the following holds:*

1. $M_k(G) \leq M_k(Y_n)$ *for all* $k \geq 0$, *and* $M_k(G) < M_k(Y_n)$ *for some* $k_0 \geq 0$.

2. $M_k(G) \leq M_k(\tilde{Y}_n)$ *for all* $k \geq 0$, *and* $M_k(G) < M_k(\tilde{Y}_n)$ *for some* $k_0 \geq 0$.

Proof. Follows from Lemma 3.1, Theorems 3.2 and 3.3, and Lemma 3.4 in [5]. □

Theorem 4. *Let G be a bicyclic graph on $n \geq 5$ vertices. Then $ER(G) \leq ER(Y_n)$, with equality if and only if $G \cong Y_n$.*

Proof. By Lemma 4, a graph with maximum resolvent energy among n-vertex bicyclic graphs is either Y_n or $\tilde{Y}_n$. Thus, it is sufficient to show that $ER(Y_n) > ER(\tilde{Y}_n)$, for $n \geq 5$. Let $\phi(Y_n, \lambda)$ and $\phi(\tilde{Y}_n, \lambda)$ denote the characteristic polynomials of Y_n and $\tilde{Y}_n$, respectively. Then, by [3, Theorem 8], we have

$$ER(Y_n) = \frac{\phi'(Y_n, n)}{\phi(Y_n, n)} \qquad \text{and} \qquad ER(\tilde{Y}_n) = \frac{\phi'(\tilde{Y}_n, n)}{\phi(\tilde{Y}_n, n)} \, .$$

By Lemma 2, it follows that

$$\begin{aligned} \phi(Y_n, \lambda) &= \lambda^{n-4}\left[\lambda^4 - (n+1)\lambda^2 - 4\lambda + 2(n-4)\right] \\ \phi(\tilde{Y}_n, \lambda) &= \lambda^{n-4}\left[\lambda^4 - (n+1)\lambda^2 + 3(n-5)\right] . \end{aligned}$$

Hence

$$\begin{aligned} ER(Y_n) - ER(\tilde{Y}_n) &= \frac{\phi'(Y_n, n)}{\phi(Y_n, n)} - \frac{\phi'(\tilde{Y}_n, n)}{\phi(\tilde{Y}_n, n)} \\ &= \frac{\phi'(Y_n, n)\,\phi(\tilde{Y}_n, n) - \phi'(\tilde{Y}_n, n)\,\phi(Y_n, n)}{\phi(Y_n, n)\,\phi(\tilde{Y}_n, n)} \\ &= \frac{16n^4 - 34n^3 + 8n^2 + 2n + 60}{(n^4 - n^3 - n^2 - 2n - 8)(n^4 - n^3 - n^2 + 3n - 15)} \, . \end{aligned}$$

The polynomial $p(x) = 16x^4 - 34x^3 + 8x^2 + 2x + 60$ does not have any real roots, thus the numerator $p(n)$ is positive for all n. The real roots of the polynomials $x^4 - x^3 - x^2 - 2x - 8$ and $x^4 - x^3 - x^2 + 3x - 15$ are less than 3, so the denominator is positive for $n \geq 3$. It follows that $ER(Y_n) - ER(\tilde{Y}_n) > 0$. □

4 Tricyclic graphs with maximum resolvent energy

Let Z_n^i, $1 \le i \le 6$, be the graphs given in Figure 3.

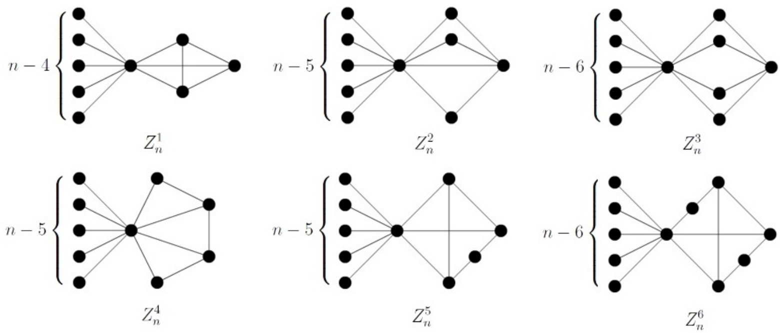

Figure 3: Tricyclic graphs with maximum resolvent energy.

Lemma 5. *Let G be a bicyclic graph on $n \ge 4$ vertices such that $G \ncong Z_n^i$, for $1 \le i \le 6$. Then, some $i \in \{1,2,3,4,5,6\}$, $M_k(G) \le M_k(Z_n^i)$ for all $k \ge 0$, and $M_k(G) < M_k(Z_n^i)$ for some $k_0 \ge 0$.*

Proof. Follows from Corollaries 3.5 and 3.9 and Lemma 3.10 in [6]. □

Theorem 5. *Let G be a tricyclic graph on $n \ge 4$ vertices. Then $ER(G) \le ER(Z_n^1)$, with equality if and only if $G \cong Z_n^1$.*

Proof. By Lemma 5, a graph with maximum resolvent energy among n-vertex tricyclic graphs is equal to Z_n^i, for some $1 \le i \le 6$.

By Lemma 2, it follows that

$$\begin{aligned}
\phi(Z_n^1,\lambda) &= \lambda^{n-5}\,(\lambda^5-(n+2)\lambda^3-8\lambda^2+3(n-5)\lambda+2(n-4)) = \lambda^{n-5}\,f_1(\lambda)\\
\phi(Z_n^2,\lambda) &= \lambda^{n-4}\,(\lambda^4-(n+2)\lambda^2-6\lambda+3(n-5)) = \lambda^{n-4}\,f_2(\lambda)\\
\phi(Z_n^3,\lambda) &= \lambda^{n-4}\,(\lambda^4-(n+2)\lambda^2+4(n-6)) = \lambda^{n-4}\,f_3(\lambda)\\
\phi(Z_n^4,\lambda) &= \lambda^{n-6}\,(\lambda^6-(n+2)\lambda^4-6\lambda^3+3(n-4)\lambda^2+2\lambda-(n-5)) = \lambda^{n-6}\,f_4(\lambda)
\end{aligned}$$

$$\begin{aligned}
\phi(Z_n^5,\lambda) &= \lambda^{n-5}\,(\lambda^5-(n+2)\lambda^3-4\lambda^2+4(n-4)\lambda+4)=\lambda^{n-5}\,f_5(\lambda)\\
\phi(Z_n^6,\lambda) &= \lambda^{n-6}\,(\lambda^6-(n+2)\lambda^4+5(n-5)\lambda^2-2(n-8))=\lambda^{n-6}\,f_6(\lambda)\,.
\end{aligned}$$

For $2 \leq i \leq 6$, we have

$$\begin{aligned}
ER(Z_n^1)-ER(Z_n^i) &= \frac{\phi'(Z_n^1,n)}{\phi(Z_n^1,n)}-\frac{\phi'(Z_n^i,n)}{\phi(Z_n^i,n)}\\
&= \frac{\phi'(Z_n^1,n)\,\phi(Z_n^i,n)-\phi'(Z_n^i,n)\,\phi(Z_n^1,n)}{\phi(Z_n^1,n)\,\phi(Z_n^i,n)}\,.
\end{aligned}$$

Straightforward calculation yields

$$\begin{aligned}
ER(Z_n^1)-ER(Z_n^2) &= \frac{6n^6-12n^5+42n^4-18n^3-42n-120}{n\,f_1(n)\,f_2(n)}\\
ER(Z_n^1)-ER(Z_n^3) &= \frac{28n^6-56n^5+44n^4-8n^3+136n^2+80n-192}{n\,f_1(n)\,f_3(n)}\\
ER(Z_n^1)-ER(Z_n^4) &= \frac{6n^8+40n^6-2n^5-48n^4-96n^3-188n^2-132n-40}{n\,f_1(n)\,f_4(n)}\\
ER(Z_n^1)-ER(Z_n^5) &= \frac{16n^7-20n^6+56n^5-40n^4+4n^3-52n^2-188n}{n\,f_1(n)\,f_5(n)}\\
ER(Z_n^1)-ER(Z_n^6) &= \frac{32n^8-62n^7+30n^6+92n^5+94n^4-2n^3-432n^2-432n-128}{n\,f_1(n)\,f_6(n)}\,.
\end{aligned}$$

All the real roots of the polynomials that appear in the numerators are less than 2. Moreover, all the real roots of the polynomials f_i, $1 \leq i \leq 6$, are less than 3. It follows that the numerator end denominator in the quotients above are positive for $n \geq 3$. Hence $ER(Z_n^1) - ER(Z_n^i) > 0$ for $2 \leq i \leq 6$. □

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