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Resolvent Energy

Ivan Gutman[1,2], **Boris Furtula**[1], **Emir Zogić**[2], **Edin Glogić**[2]

[1] *Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*
gutman@kg.ac.rs, furtula@kg.ac.rs

[2] *State University of Novi Pazar, Novi Pazar, Serbia*
ezogic@np.ac.rs, edinglogic@np.ac.rs

1 Introduction

Let $\mathbf{M}$ be a square matrix of order n. In linear algebra, the *resolvent matrix* $\mathcal{R}_{\mathbf{M}}(z)$ of $\mathbf{M}$ plays an important role [21]. It is defined as

$$\mathcal{R}_{\mathbf{M}}(z) = \big(z\,\mathbf{I}_n - \mathbf{M}\big)^{-1}$$

where $\mathbf{I}_n$ is the unit matrix of order n and z a complex variable. As easily seen, $\mathcal{R}_{\mathbf{M}}(z)$ is also a matrix of order n, that exists for all values of z except when z coincides with an eigenvalue of $\mathbf{M}$.

In this paper, we are concerned with simple graphs, that is graphs without directed, multiple, or weighted edges, and without self–loops. Let G be such a graph, possessing n vertices and m edges, and let $\mathbf{A} = \mathbf{A}(G)$ be its $(0,1)$-adjacency matrix.

Since $\mathbf{A}$ is a real and symmetric matrix of order n, its eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ are real numbers. These eigenvalues form the spectrum of G [6, 7].

The k-th spectral moment of the graph G is defined as

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k \ . \tag{1}$$

As well known [6,7], $M_0 = n$, $M_1 = 0$, $M_2 = 2m$, and $M_k = 0$ for all odd values of k if and only if G is bipartite.

The resolvent matrix of $\mathbf{A}(G)$ is

$$\mathcal{R}_{\mathbf{A}}(z) = \big(z\,\mathbf{I}_n - \mathbf{A}\big)^{-1}$$

and its eigenvalues are

$$\frac{1}{z-\lambda_i}\ , \quad i = 1, 2, \ldots, n\,. \tag{2}$$

The energy of the graph G is defined as the sum of absolute values of its eigenvalues, i.e.,

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|\,. \tag{3}$$

This spectrum–based graph invariant was introduced in the 1970s [10]. Since then, its theory has been extensively elaborated [18] resulting in several hundreds of published papers [12]. Also a number of other "graph energies" have been introduced, based on matrices other than $\mathbf{A}(G)$ [11,18].

Bearing in mind the expressions (2), in analogy with Eq. (3), one could think of defining a "*resolvent graph energy*" as [15]

$$\sum_{i=1}^{n} \left| \frac{1}{z-\lambda_i} \right|$$

that would then depend on the complex variable z and would not exist for $z = \lambda_i$, $i = 1, 2, \ldots, n$.

In order to ameliorate the above ill-defined "resolvent–energy" concept, taking into account that that the condition $\lambda_i \leq n-1$ is satisfied by all eigenvalues of all n-vertex graphs [6,7], we propose the choice $z = n$. Thus we define the *resolvent energy* of a graph G as follows:

Definition 1. [15] *Let G be a graph on n vertices with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. Its resolvent energy is*[1]

$$ER = ER(G) = \sum_{i=1}^{n} \frac{1}{n-\lambda_i}\,. \tag{4}$$

Note that the term $\frac{1}{n-\lambda_i}$, occurring on the right–hand side of Eq. (4), is always positive–valued.

[1]Resolvent energy had to be denoted by ER, because RE is nowadays used for "Randić energy" [2,8,17].

The resolvent energy, introduced via Definition 1, is similar to, but not identical with, an earlier studied spectrum–based graph invariant, put forward by Estrada and Higham [16] and defined as

$$EE_r = EE_r(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{(n-1)^k} \,. \tag{5}$$

Its relation to the resolvent of the adjacency matrix was recognized by Benzi and Boito [1], by showing that

$$EE_r = \sum_{i=1}^{n} \frac{n-1}{n-1-\lambda_i} \tag{6}$$

in view of which EE_r has been named "resolvent Estrada index". Note that according to Eq. (6), EE_r is undefined (i.e., infinite) in the case of the complete graph K_n .

Additional properties of EE_r can be found in the recent papers [3, 4, 13, 14].

2 Basic Properties of Resolvent Energy

Theorem 2. *If G is a graph of order n and $M_k(G)$, $k = 0, 1, 2, \ldots$ its spectral moments, Eq. (1), then*

$$ER(G) = \frac{1}{n} \sum_{k=0}^{\infty} \frac{M_k(G)}{n^k} \,. \tag{7}$$

Proof. Starting with Definition 1, and bearing in mind that $|\lambda_i/n| < 1$, we have

$$ER(G) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{1-\frac{\lambda_i}{n}} = \frac{1}{n} \sum_{i=1}^{n} \sum_{k=0}^{\infty} \left(\frac{\lambda_i}{n}\right)^k = \frac{1}{n} \sum_{k=0}^{\infty} \sum_{i=1}^{n} \left(\frac{\lambda_i}{n}\right)^k = \frac{1}{n} \sum_{k=0}^{\infty} \frac{1}{n^k} \sum_{i=1}^{n} (\lambda_i)^k$$

and the relation (7) follows from Eq. (1). ■

Formula (7) should be compared with Eq. (5).

The k-th spectral moment is equal to the number of self-returning walks of length k [6, 7]. Therefore, by deleting an edge from the graph G, each spectral moment will diminish or remain unchanged. At least M_2 will strictly diminish. In view of this, Eq. (7) immediately implies:

Corollary 3. *If e is a edge of the graph G, denote by $G-e$ the subgraph obtained by deleting e from G. Then for any edge e of G,*

$$ER(G-e) < ER(G) \,.$$

Corollary 4. *Let K_n be the complete graph of order n and $\overline{K}_n$ the edgeless graph of order n. Then for any graph G of order n, different from K_n and $\overline{K}_n$,*

$$ER(\overline{K}_n) < ER(G) < ER(K_n)\,.$$

As well known [6, 7], the spectra of K_n and $\overline{K}_n$ are $\{n-1,-1,-1,\dots,-1\}$ and $\{0,0,\dots,0\}$, respectively. Then from Corollary 4 it follows:

Corollary 5. *If G is a graph of order n, then*

$$1 \leq ER(G) \leq \frac{2n}{n+1}\,.$$

Equality $ER(G)=1$ holds if and only if $G \cong \overline{K}_n$. Equality $ER(G)=\frac{2n}{n+1}$ holds if and only if $G \cong K_n$.

Corollary 6. *Among connected graphs of order n, the graph with smallest resolvent energy is a tree.*

Let, as usual, P_n and S_n denote the path and star on n vertices.

Theorem 7. *Among trees of order n, the path P_n has smallest and the star S_n has greatest resolvent energy.*

Proof. Recall first that since trees are bipartite graphs, all their odd spectral moments are equal to zero.

In the paper [9], Hanyuan Deng proved that for P_n and S_n being the n-vertex path and star, and T being any other tree of the same order, the inequalities

$$M_{2k}(P_n) \leq M_{2k}(T) \leq M_{2k}(S_n)$$

hold for all k. It is easy to verify that for $k \geq 2$, $M_{2k}(P_n) < M_{2k}(T) < M_{2k}(S_n)$. These results, combined with Eq. (7), directly imply Theorem 7. ■

The characteristic polynomial of the graph G is defined as [6, 7]

$$\phi(G,\lambda) = \det\left[\lambda\,\mathbf{I}_n - \mathbf{A}(G)\right].$$

Theorem 8. *Let G be a graph of order n. Then*

$$ER(G) = \frac{\phi'(G,n)}{\phi(G,n)} \tag{8}$$

where $\phi'(G,\lambda)$ is the first derivative of $\phi(G,\lambda)$.

Proof. Eq. (8) follows from the definition (4), by taking into account

$$\phi(G,\lambda) = \prod_{i=1}^{n} (\lambda - \lambda_i)\,.$$

■

Formula (8) is interesting because it shows that the resolvent energy can be calculated without knowing the graph eigenvalues. Because the coefficients of the characteristic polynomial are integers, Eq. (8) implies that ER is always a rational number.

3 Estimating the Resolvent Energy

We start by stating two lemmas that are needed in the forthcoming discussion.

Lemma 9. [7] *A graph has one eigenvalue if and only if it is totally disconnected. A graph has two distinct eigenvalues $\lambda_1 > \lambda_2$ with multiplicities m_1 and m_2 if and only if it consists of m_1 complete graphs of order $\lambda_1 + 1$. In that case, $\lambda_2 = -1$ and $m_2 = m_1\,\lambda_1$.*

Lemma 10. [20] *For real numbers $a_1 \geq a_2 \geq \cdots \geq a_k \geq 0$ and $\alpha > 1$,*

$$\sum_{i=1}^{k} (a_i)^\alpha \leq \left(\sum_{i=1}^{k} a_i \right)^\alpha$$

with equality if and only if $a_2 = a_3 = \cdots = a_k = 0$.

Theorem 11. [15] *Let G be a graph with n vertices and m edges. Then*

$$\frac{n^3}{n^3 - 2m} \leq ER(G) \leq 1 + \frac{2m(2n-1)}{n^2\,(n^2 - 2m)}\,. \tag{9}$$

Equality on the left–hand side is attained if and only if $G \cong \overline{K}_n$ or (provided n is even) $G \cong \frac{n}{2}\,K_2$. Equality on the right–hand side is attained if and only if $G \cong \overline{K}_n$.

Proof.

1. Lower bound in (9). According to Eq. (4),

$$ER = \frac{1}{n}\sum_{k\geq 0}\frac{M_k}{n^k} \geq \frac{1}{n}\sum_{k\geq 0}\frac{M_{2k}}{n^{2k}}$$

with equality if and only if G is bipartite. Further,

$$\begin{aligned}\frac{1}{n}\sum_{k\geq 0}\frac{M_{2k}}{n^{2k}} &= \frac{1}{2n}\left[\sum_{k\geq 0}\frac{M_k}{n^k}+\sum_{k\geq 0}(-1)^k\frac{M_k}{n^k}\right] = \frac{1}{2n}\left[\sum_{i=1}^{n}\frac{1}{1-\frac{\lambda_i}{n}}+\sum_{i=1}^{n}\frac{1}{1+\frac{\lambda_i}{n}}\right]\\ &= \frac{1}{n}\sum_{i=1}^{n}\frac{1}{1-\left(\frac{\lambda_i}{n}\right)^2} \geq \frac{1}{n}\frac{n^2}{\sum\limits_{i=1}^{n}\left(1-\left(\frac{\lambda_i}{n}\right)^2\right)}\end{aligned} \tag{10}$$

where we used a special case of the Cauchy–Schwarz inequality, namely

$$\sum_{i=1}^{n}\frac{1}{x_i} \geq \frac{n^2}{\sum\limits_{i=1}^{n}x_i}$$

in which equality is attained if and only if $x_1 = x_2 = \cdots = x_n$.

The expression on the right–hand side of (10) is now transformed into

$$\frac{1}{n}\frac{n^4}{\sum\limits_{i=1}^{n}\left(n^2-\lambda_i^2\right)} = \frac{n^3}{n^3-\sum\limits_{i=1}^{n}(\lambda_i)^2}$$

which in view of $M_2 = 2m$ leads to the lower bound in (9).

Equality is attained if and only if the graph G is bipartite and if its eigenvalues satisfy the condition $\lambda_1^2 = \lambda_2^2 = \cdots = \lambda_n^2$. By Lemma 9 we conclude that $G \cong \overline{K}_n$ or $G \cong \frac{n}{2}\,K_2$ (provided n is even).

2. Upper bound in (9). We start again with Eq. (4), and recall that $M_0 = n$ and $M_1 = 0$. Then,

$$\begin{aligned}ER &= \frac{1}{n}\left[\sum_{k\geq 0}\frac{M_{2k}}{n^{2k}}+\sum_{k\geq 0}\frac{M_{2k+1}}{n^{2k+1}}\right] = \frac{1}{n}\left[n+\sum_{k\geq 1}\frac{M_{2k}}{n^{2k}}+\sum_{k\geq 1}\frac{M_{2k+1}}{n^{2k+1}}\right]\\ &= 1+\frac{1}{n}\sum_{k\geq 1}\left[\frac{\sum\limits_{i=1}^{n}(\lambda_i)^{2k}}{n^{2k}}+\frac{\sum\limits_{i=1}^{n}(\lambda_i)^{2k+1}}{n^{2k+1}}\right]\\ &\leq 1+\frac{1}{n}\sum_{k\geq 1}\left[\frac{\sum\limits_{i=1}^{n}(\lambda_i)^{2k}}{n^{2k}}+\frac{n-1}{n}\frac{\sum\limits_{i=1}^{n}(\lambda_i)^{2k}}{n^{2k}}\right]\end{aligned} \tag{11}$$

where the fact $n-1 \geq \lambda_i$ has been used.

Equality happens only if $\lambda_i = 0$ or $\lambda_i = n-1$ $(i = 1, 2, \ldots, n)$, i.e., if and only if $G \cong \overline{K}_n$.

The expression on the right–hand side of (11) is now transformed into

$$\begin{aligned} 1 + \frac{1}{n} \cdot \frac{2n-1}{n} \sum_{k \geq 1} \frac{\sum_{i=1}^{n} (\lambda_i)^{2k}}{n^{2k}} &\leq 1 + \frac{2n-1}{n^2} \sum_{k \geq 1} \left(\frac{\sum_{i=1}^{n} (\lambda_i)^2}{n^2} \right)^k \\ = \quad 1 + \frac{2n-1}{n^2} \sum_{k \geq 1} \left(\frac{2m}{n^2} \right)^k &= 1 + \frac{2n-1}{n^2} \left[\sum_{k \geq 0} \left(\frac{2m}{n^2} \right)^k - 1 \right] \\ = \quad 1 + \frac{2n-1}{n^2} \left(\frac{1}{1 - \frac{2m}{n^2}} - 1 \right) & \end{aligned}$$

which straightforwardly leads to the upper bound in (9).

By Lemma 10, equality is attained if and only if $G \cong \overline{K}_n$. ■

If we possess the information about the nullity (= number of zero eigenvalues) of the graph G, then the lower bound in (9) can be improved.

Proposition 12. [15] *Let G be a graph with n vertices, m edges, and nullity n_0. Then*

$$ER(G) \geq \frac{n_0}{n} + \frac{n(n-n_0)^2}{n^2(n-n_0) - 2m}. \tag{12}$$

Proof. In the proof of Theorem 11 it was shown that $ER \geq \frac{1}{n} \sum_{i=1}^{n} \frac{1}{1 - \left(\frac{\lambda_i}{n}\right)^2}$. Denoting by $\sum_{\lambda \neq 0}$ summation over non-zero eigenvalues, we get

$$\begin{aligned} ER \quad &\geq \quad \frac{n_0}{n} + \frac{1}{n} \sum_{\lambda \neq 0} \frac{1}{1 - \left(\frac{\lambda_i}{n}\right)^2} \\ &\geq \quad \frac{n_0}{n} + \frac{1}{n} \frac{(n-n_0)^2}{\sum_{\lambda \neq 0} \left(1 - \left(\frac{\lambda_i}{n}\right)^2\right)} = \frac{n_0}{n} + \frac{1}{n} \cdot \frac{(n-n_0)^2}{n - n_0 - \frac{2m}{n^2}} \end{aligned}$$

from which inequality (12) directly follows. ■

If G is a bipartite graph with odd number of vertices, then $n_0 \geq 1$ [5]. For such graphs,

$$ER(G) \geq \frac{1}{n} + \frac{n(n-1)^2}{n^2(n-1) - 2m}.$$

If the graph G is bipartite, then the upper bound in (9) can be somewhat improved.

Proposition 13. [15] *Let G be a bipartite graph with n vertices and m edges. Then*

$$ER(G) \leq 1 + \frac{2m}{n(n^2 - m)} \, . \tag{13}$$

Equality is attained if and only if either $G \cong \overline{K}_n$ or $G \cong K_{a,b} \cup \overline{K}_{n-a-b}$, where $K_{a,b}$ is a complete bipartite graph such that $ab = m$.

Proof. Since G is bipartite, then $M_{2k+1}(G) = 0$ for all $k \geq 0$ and $\sum_{+} \lambda_i^2 = m$, where $\sum_{+}$ indicates summation over all positive eigenvalues of the corresponding graph. By using Lemma 10, assuming that $n \geq 3$, we have

$$\begin{aligned} ER &= \frac{1}{n} \sum_{k \geq 0} \frac{M_{2k}}{n^{2k}} = 1 + \frac{1}{n} \sum_{k \geq 1} \frac{\sum_{i=1}^{n} (\lambda_i)^{2k}}{n^{2k}} \\ &= 1 + \frac{2}{n} \sum_{k \geq 1} \frac{\sum_{+} (\lambda_i^2)^k}{(n^2)^k} \leq 1 + \frac{2}{n} \sum_{k \geq 1} \left(\frac{\sum_{+} (\lambda_i)^2}{n^2} \right)^k \\ &= 1 + \frac{2}{n} \sum_{k \geq 1} \left(\frac{m}{n^2} \right)^k = 1 + \frac{2}{n} \left[\sum_{k \geq 0} \left(\frac{m}{n^2} \right)^k - 1 \right] = 1 + \frac{2}{n} \left(\frac{1}{1 - \frac{m}{n^2}} - 1 \right) \end{aligned}$$

which straightforwardly leads to (13).

The equality in (13) is attained if and only if G has no more than one positive eigenvalue. If G has no positive eigenvalue, then all its eigenvalues are equal to zero, which implies that G is the empty graph $\overline{K}_n$. If G has exactly one positive eigenvalue, then by Lemma 9, and recalling that G is bipartite, G must consist of a complete bipartite graph $K_{a,b}$ and $n - a - b$ isolated vertices, where $ab = m$. ■

4 Computational Studies on Resolvent Energy

In order to gain a better insight into the properties of the resolvent energy, we have undertaken extensive computer–aided studies. The ER-values of all trees and connected unicyclic, bicyclic, and tricyclic graphs up to 15 vertices were computed, and the structure of the extremal members of these classes was established. Thus our examination embraced over ten million graphs. The main conclusions gained within these studies are the following.

First of all, the results of Theorem 7 were confirmed and extended:

Observation 14. *Consider the graphs depicted in Fig. 1. Among trees of order n, the path P_n has smallest and the tree P_n^* second–smallest resolvent energy. Among trees of order n, the star S_n has greatest and the tree S_n^* second–greatest resolvent energy.*

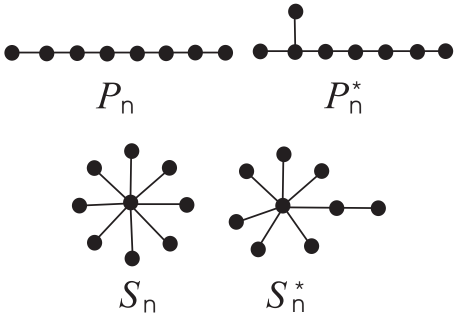

Fig. 1. Trees with extremal resolvent energy; for details see Observation 14.

Observation 15. *Consider the graphs depicted in Fig. 2. Among connected unicyclic graphs of order n, $n \geq 4$, the cycle C_n has smallest and the graph C_n^* second–smallest resolvent energy. Among these graphs of order n, $n \geq 5$, the graphs X_n and X_n^* have, respectively, greatest and second–greatest resolvent energy.*

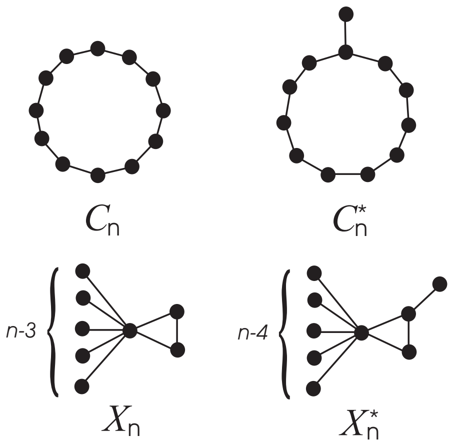

Fig. 2. Unicyclic graphs with extremal resolvent energy; for details see Observation 15.

Observation 16. *Consider the graphs depicted in Fig. 3. Among connected bicyclic graphs of order n, those with the smallest resolvent energy are:*

$$\begin{array}{lll} B_{p-1,p-1,p} & \textit{if} & n=3p\,,\ p\geq 2 \\ B_{p-1,p,p} & \textit{if} & n=3p+1\,,\ p\geq 1 \\ B_{p,p,p} & \textit{if} & n=3p+2\,,\ p\geq 1\,. \end{array} \tag{14}$$

The graphs with second–smallest resolvent energy are

$$\begin{array}{lll} B_{p-2,p,p} & \textit{if} & n=3p\,,\ p\geq 2 \\ B_{p-1,p-1,p+1} & \textit{if} & n=3p+1\,,\ p\geq 2 \\ B_{p-1,p,p+1} & \textit{if} & n=3p+2\,,\ p\geq 1\,. \end{array}$$

Among these graphs of order n, $n \geq 5$, the graph Y_n has greatest resolvent energy. For $n \geq 9$, the graph Y_n^* has second–greatest resolvent energy, whereas Y_5^*, Y_6^*, Y_7^*, and Y_8^* are exceptions.

Observation 17. *Consider the graphs depicted in Fig. 4. Among connected tricyclic graphs of order n, $n \geq 5$, the graph Z_n has greatest resolvent energy. For $n \geq 6$, the graph Z_n^* has second–greatest resolvent energy, whereas Z_5^* is an exception.*

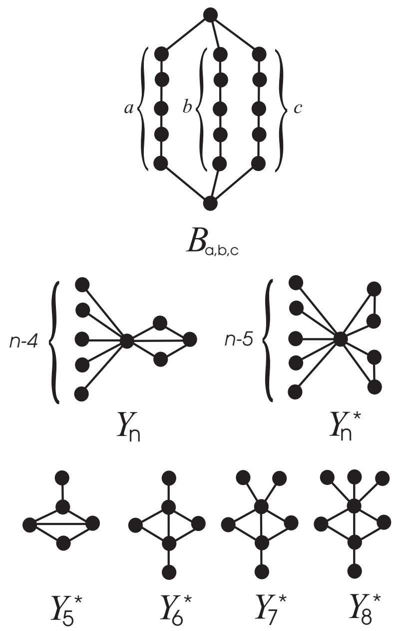

Fig. 3. Bicyclic graphs with extremal resolvent energy; for details see Observation 16.

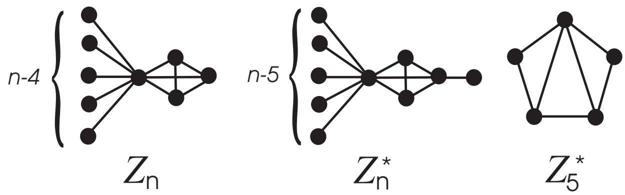

Fig. 4. Tricyclic graphs with greatest resolvent energy; for details see Observation 17.

Observation 18. *The structural regularity obeyed by the connected tricyclic graphs with smallest ER is not easy to envisage. These graphs of order* n , $5 \leq n \leq 15$, *are depicted in Fig. 5.*

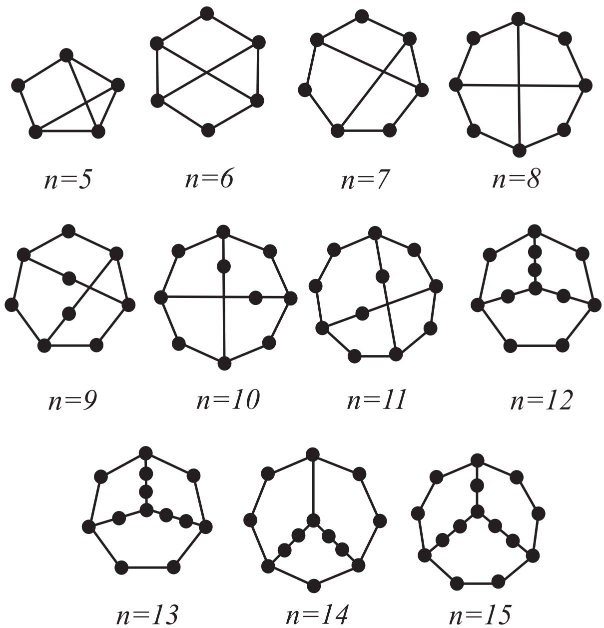

Fig. 5. Tricyclic graphs of order n , $5 \leq n \leq 15$, with smallest resolvent energy.

Observation 19. *The inequality* $ER(S_n) < ER(C_n)$ *holds for all* $n \geq 4$. *Consequently, any tree has smaller ER-value than any unicyclic graph of the same order.*

For $B_{a,b,c}$ *specified by Eq. (14), the inequality* $ER(X_n) < ER(B_{a,b,c})$ *holds only until* $n = 6$ *and is violated for all* $n \geq 7$. *Consequently, it is not true that any unicyclic graph has smaller ER-value than any bicyclic graph of the same order. The same applies also to the relation between ER of bicyclic and tricyclic graphs. On the other hand, any unicyclic graph has smaller ER-value than any connected tricyclic graph of the same order.*

Observation 20. *Evidently, cospectral graphs have equal* ER*-values. Until now, we did not detect pairs of (connected) non-cospectral graphs with equal* ER*-values. However, there exist non-cospectral graphs whose* ER*-values are different, but remarkably close. For instance,* $ER(B_{3,3,3}) = 1.018571022$ *whereas* $ER(B_{2,3,4}) = 1.018571080$*, and* $ER(B_{4,4,5}) = 1.0096261837436$ *whereas* $ER(B_{3,5,5}) = 1.0096261837458$*. These findings resemble the existence of the earlier discovered almost–equienergetic graphs* [19, 22, 23].

5 Summary and Conclusion

In this paper, we established a number of properties of the resolvent energy ER. A few of these were proven by mathematical arguments and stated as Theorems 2, 7, 8, 11 and their corollaries. Additional results, stated here as Observations 14–20, should be considered as conjectures, awaiting to be verified or (what we deem to be less likely) refuted. We believe that these will invite other colleagues to undertake additional research of this newly conceived graph–spectrum–based structure descriptor.

Another topic that calls for investigation are the relations between the ordinary graph energy E, Eq. (3), and ER, Eq. (4). In order that ER gets applications independent of E (especially in chemistry–related fields), of paramount importance would be to have cases in which structure–dependence of ER is significantly different from that of E. In our future studies, we intend to pay particular attention on discovering and characterizing such properties of the resolvent energy.

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