TAMKANG JOURNAL OF MATHEMATICS
Volume 45, Number 4, 375-387, December 2014
doi:10.5556/j.tkjm.45.2014.1463
Available online at http://journals.math.tku.edu.tw/

ON REVISED SZEGED SPECTRUM OF A GRAPH

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Abstract. The revised Szeged index is a molecular structure descriptor equal to the sum of products $[n_u(e)+\frac{n_0(e)}{2}][n_v(e)+\frac{n_0(e)}{2}]$ over all edges $e = uv$ of the molecular graph G, where $n_0(e)$ is the number of vertices equidistant from u and v, $n_u(e)$ is the number of vertices closer to u than v and $n_v(e)$ is defined analogously. The adjacency matrix of a graph weighted in this way is called its revised Szeged matrix and the set of its eigenvalues is the revised Szeged spectrum of G. In this paper some new results on the revised Szeged spectrum of graphs are presented.

1. Introduction

A *topological index* is an applicable graph invariant in chemistry. Such numbers are studied in structure-property and structure-activity studies. To explain, we assume that $Graph$ denotes the set of all finite connected graphs. A map Top from $Graph$ into real numbers is called a topological index if G is isomorphic to H then $Top(G) = Top(H)$. The first of such graph invariants is Wiener index [15] which is defined as the summation of all distances between vertices of the graph under consideration. Here, for two vertices x and y of the graph G, the distance $d_G(x, y)$ is the length of a minimal path connecting them.

In [8], Ivan Gutman introduced a generalization of the original Wiener index which is called "Szeged index". Suppose G is a connected graph. The Szeged index, $Sz(G)$, is defined as $Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e)$, where $n_u(e)$ is the number of vertices closer to u than v and $n_v(e)$ is defined analogously. This topological index found applications in QSPR studies and its mathematical properties have been extensively studied [6, 7, 11]. Milan Randić [14] introduced a Wiener-Szeged type topological index as a modification of Szeged index. In recent years, the authors prefer to use the name revised Szeged index for this topological index. The revised Szeged index is defined by the following formula:

$$Sz^\star(G) = \sum_{e=uv\in E(G)} \left(n_u(e)+\frac{n_0(e)}{2}\right)\left(n_v(e)+\frac{n_0(e)}{2}\right).$$

Received July 20, 2013, accepted April 15, 2014.
2010 *Mathematics Subject Classification*. 05C35, 05C12, 05C05.
Key words and phrases. Revised Szeged index, Revised Szeged matrix spectrum.
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where $n_0(e)$ is the number of vertices equidistant from both end-vertex of edge $e = uv$. Some mathematical properties of this graph invariant are reported in [3, 12, 13, 16].

In this paper, we continue the lines [4] to define a new weighting of graphs and the eigenvalues of the associated adjacency and Laplacian matrices by using the revised Szeged index. The functions $w, w' : E(G) \longrightarrow R$, where $w(e) = n_u(e)n_v(e)$ and $w'(e) = [n_u(e)+\frac{1}{2}n_0(v)][n_v(e)+\frac{1}{2}n_0(v)]$ for $e = uv$, are weight functions on the edge set $E(G)$. We call these weight functions, the Szeged and revised Szeged weighting, respectively. For terms and concepts not defined here we refer the reader to [1, 2, 5, 9].

2. Definitions and examples

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. The adjacency matrix of G is denoted by $A(G)$ and its eigenvalues are called eigenvalues of the graph G. It is clear that the product $(n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2})$ is always positive, and the function $Sz^\star : E(G) \to \mathbb{R}^+$ given by $Sz^\star(e) = (n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2})$ is a weight function on $E(G)$. We call this weight function the revised Szeged weighting of G. The adjacency matrix of a graph G weighted by the revised Szeged weighting is called the revised Szeged matrix of G and denoted by $Sz^\star M(G) = [s_{i,j}]$. The eigenvalues of this matrix are called the revised Szeged eigenvalues of G and denoted by $\sigma_r(G)$, for $r = 1,\ldots,n$. Obviously, the revised Szeged index of a graph G can be expressed as one half of the sum of all entries of $Sz^* M(G)$.

Let G be a weighted graph with a weight function $w : E(G) \to \mathbb{R}^+$ and $W(G) = [w_{i,j}]$ its adjacency matrix. Here $w(uv) = w(vu)$ and hence $w_{i,j} = w_{j,i}$. The Laplacian matrix of a weighted graph G is defined as $LW(G) = [l_{i,j}]$, where

$$l_{ij} = \begin{cases} \sum_{k=1}^n w_{ik} & i = j \\ -w_{ij} & ij \in E(G) \\ 0 & o.w \end{cases}$$

The Laplacian matrix of G is defined as $L(G) = D(G) - A(G)$, where $D(G)$ is a diagonal matrix whose (i,i)-entry is $\deg(v_i)$, the degree of vertex v_i. Similar to [4], we denote the Laplacian matrix of a graph G weighted by the revised Szeged weighting by $LSz^\star M(G)$ which is called the Laplacian revised Szeged matrix of G . The eigenvalues of this matrix are the Laplacian revised Szeged eigenvalues of G, denoted by $\mu_r^{'}(G)$, $r = 1,\ldots,n$, while the eigenvalues of the Laplacian matrix of the underlying unweighted graph G are denoted by $\mu_r(G)$, $r = 1,\ldots,n$.

Example 2.1. Suppose that K_n denotes the complete graph with n vertices. Then for an edge $e = uv$, $n_u(e) = n_v(e) = 1$ and $n_0(e) = n-2$. So,

$$Sz^\star(e) = (n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2})$$

$$= (1 + \frac{n-2}{2})(1 + \frac{n-2}{2}) = \frac{n^2}{4}.$$

Thus $Sz^\star M(K_n) = (\frac{n}{2})^2 A(G)$. So, $\sigma_r(K_n) = (\frac{n}{2})^2 \lambda(K_n)$ and revised Szeged eigenvalues of K_n are $\frac{n^2(n-1)}{4}$ and $\frac{(-1)n^2}{4}$ with multiplicity 1 and $n-1$, respectively. Hence, the revised Szeged Laplacian eigenvalues of K_n are $\frac{n^2(n-1)}{2}$ and 0 with multiplicity 1 and $n-1$, respectively.

Example 2.2. Let C_n be the cycle graph on n vertices. It is well−known that the spectrum of C_n is given by $\lambda_r(C_n) = 2\cos(\frac{2r\pi}{n})$, see [2, p.72] for details. Since $L(C_n) = 2I - A(C_n)$, the Laplacian eigenvalues are given by $\mu_r(C_n) = 4\sin^2(\frac{2r\pi}{n})$. It is easy to verify that for each edge $e = uv$ of C_n, the product

$$(n_u(e) + \frac{n_0(e)}{2})(n_v(e) + \frac{n_0(e)}{2}) = \frac{n^2}{4}$$

does not depend to parity of n and that it is given by

$$Sz^\star M(C_n) = (\frac{n^2}{4})A(C_n) \quad \text{and} \quad LSz^\star M(C_n) = (\frac{n^2}{4})L(C_n).$$

Thus

$$\sigma_r(C_n) = \frac{n^2}{2}\cos(\frac{2r\pi}{n}) \quad \text{and} \quad \mu'_r(C_n) = n^2\sin^2(\frac{r\pi}{n}).$$

Example 2.3. Let $K_{m,n}$ be the complete bipartite graph. Since the revised Szeged weighting of any edge is mn, we have

$$Sz^* M(K_{m,n}) = mnA(K_{m,n}) \quad \text{and} \quad LSz^* M(K_{m,n}) = mnL(K_{m,n}).$$

Therefore,

$$\sigma_r(K_{m,n}) = mn\lambda_r(K_{m,n}) \quad \text{and} \quad \mu'_r(K_{m,n}) = mn\mu_r(K_{m,n}).$$

From the Laplacian spectrum of $K_{m,n}$, one can see that the Laplacian revised Szeged eigenvalues of $K_{m,n}$ are 0 and $mn(m+n)$ with multiplicity one, m^2n with multiplicity $n-1$ and mn^2 with multiplicity $m-1$. In particular, for $m = n$, one obtains 0, n^3 and $2n^3$ as the Laplacian revised Szeged eigenvalues of K_n, with given multiplicities.

3. Main result

A graph G in which for every edge $e = uv$, $n_u(e) = n_v(e)$ is called *distance-balanced* [10]. Suppose G is connected and $e = uv$ is an edge of G. Define:

$$N_u(e) = \{w \in V(G) | d(u,w) - d(v,w) = -1\},$$

$$N_v(e) = \{w \in V(G) | d(u,w) - d(v,w) = 1\},$$

$$N_0(e) = \{w \in V(G) | d(u,w) - d(v,w) = 0\}.$$

It is easy to see that $N_u(e), N_v(e)$ and $N_0(e)$ constitutes a partition for $V(G)$ and $n_u(e) + n_v(e) + n_0(e) = n$. On the other hand, for any edge $e = uv$,

$$\begin{aligned} Sz^*(e) &= (n_u(e) + \frac{n_0}{2})(n_v + \frac{n_0}{2}) \\ &= (n_u + \frac{n - n_u - n_v}{2})(n_v + \frac{n - n_u - n_v}{2}) \\ &= \frac{n + n_u - n_v}{2} . \frac{n - (n_u - n_v)}{2} \\ &= \frac{n^2 - (n_u - n_v)^2}{4}. \end{aligned} \tag{*}$$

Lemma 3.1 ([16], Theorem 3.1). *Suppose G is a connected graph with n vertices and m edges. Then*

$$(n-1)m \leq Sz^\star(G) \leq \frac{n^2}{4}m,$$

with left equality if and only if $G = S_n$, and right equality if and only if G is distance-balanced.

Lemma 3.2. *Suppose that G is a connected graph on n vertices. The graph G is distance-balanced if and only if $Sz^* M(G) = \frac{n^2}{4} A(G)$.*

Proof. Suppose that G is a distance-balanced graph. Then for any edge $e = uv$, $n_0(e) = n - 2n_u$. So,

$$Sz^*(e) = (n_u + \frac{n_0}{2})(n_v + \frac{n_0}{2}) = (n_u + \frac{n - 2n_u}{2})(n_v + \frac{n - 2n_v}{2}) = (\frac{n}{2})^2.$$

Conversely, suppose that for any edge $e = uv$, $Sz^*(e) = \frac{n^2}{4}$. Then

$$(n_u + \frac{n_0}{2})(n_v + \frac{n_0}{2}) = \frac{n^2}{4}$$

On the other hand, from the relation $(*)$,

$$(n_u + \frac{n_0}{2})(n_v + \frac{n_0}{2}) = \frac{n^2 - (n_u - n_v)^2}{4}.$$

Thus, $(n_u - n_v)^2 = 0$ which implies that $n_u = n_v$. Therefore, G is distance-balanced. □

If G is vertex-transitive then G is distance-balanced and so by Lemma 3.2, $Sz^* M(G) = \frac{n^2}{4} A(G)$. Suppose $e = uv \in E(G)$. Define $S_i(w) = \{v \in V(G) | d(v, w) = i\}$, $1 \leq i \leq d$, where d is the diameter of G.

3.1. Circulant graphs

A square matrix S of order n is called circulant if $s_{ij} = s_{1,j-i+1}$, where addition is performed modulo n. From definition, it is clear that each circulant matrix can be determined fully by its first row. A circulant matrix Z is said to be in canonical form if the first row is given by $[0,1,0,\ldots,0]$. It is well-known that if S is a circulant matrix with the first row $[s_1,\ldots,s_n]$ then $S=\sum_{j=1}^{n} s_j Z^{j-1}$. Since the eigenvalues of Z are $1,\omega,\omega^2,\ldots,\omega^{n-1}$ where $\omega=\exp(\frac{2\pi i}{n})$, the spectrum of S is:

$$\lambda_r(S)=\sum_{j=1}^{n} s_j\omega^{(j-1)r},$$

for $r=1,2,\ldots,n$.

A graph G is called circulant, if its adjacency matrix is circulant. By above discussion, the eigenvalues of a circulant graph G is determined by

$$\lambda_r(G)=\sum_{j=1}^{n} a_j\omega^{(j-1)r},$$

for $r=1,2,\ldots,n$.

Clearly, the cycle graph C_n is circulant.

Proposition 3.3. *Let G be a circulant graph on n vertices. Then $Sz^*M(G)=\frac{n^2}{4}A(G)$. Furthermore, $\mu_r^\star(G)=\frac{n^2k}{4}-\sigma_r(G)$ for some k, where $\sigma_r(G)$ is the r-th revised Szeged eigenvalue of G.*

Proof. The proof follows from vertex-transitivity of circulant graphs. □

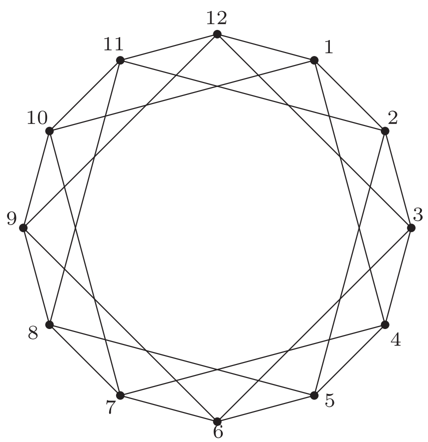

Figure 1: The Circulant Graph $C_{12,3}$.

As an application of Proposition 3.3, we calculate the revised Szeged Laplacian eigenvalues of the circulant graph $C_{n,k}$, $k\le[\frac{n}{2}]$, see Figure 1. To do this, we notice that the first row of $A(C_{n,k})$ is $[0,1,0\ldots,\overbrace{1}^{\text{(k+1)-th}},0,\ldots,0,\overbrace{1}^{\text{(n-(k-1))-th}},0,\ldots,0,1]$ and its eigenvalues are $\lambda_r(C_{n,k})=2[\cos(\frac{2r\pi}{n})+\cos(\frac{2kr\pi}{n})]$. On the other hand, the Laplacian eigenvalues of $C_{n,k}$ are $\mu(C_{n,k})=4\sin^2(\frac{r\pi}{n})+4\sin^2(\frac{kr\pi}{n})$. It is easy to see that $Sz^*M(C_{n,k})$ is a circulant matrix and its first row is:

$[0, \frac{n^2}{4}, 0\ldots, \overbrace{\frac{n^2}{4}}^{\text{(k+1)-th}}, 0, \ldots, 0, \overbrace{\frac{n^2}{4}}^{\text{(n-(k-1))-th}}, 0, \ldots, 0, \frac{n^2}{4}]$. By our discussion given above, the eigenvalues of this matrix are $\sigma_r(C_{n,2}) = \frac{n^2}{2}(\cos(\frac{2r\pi}{n}) + \cos(\frac{2kr\pi}{n})$. Finally, by applying Proposition 3.3 we obtain the following result:

Corollary 3.4. *The Laplacian revised Szeged eigenvalues of $C_{n,k}$ are given by*

$$\mu_r^{'}(C_{n,k}) = n^2(1 + \sin^2(\frac{r\pi}{n}) + \sin^2(\frac{kr\pi}{n})),$$

for $r = 1, \ldots, n$.

As the second example, we now consider the Möbius ladder with n rungs M_n. It has $2n$ vertices, see Figure 2. The eigenvalues of M_n are obtained in a similar way as circulant graphs. We consider the first row $[0, 1, 0, \ldots, 0, \overbrace{1}^{\text{n+1 th}}, 0, \ldots, 0, 1]$ of the adjacency matrix of M_n.

$$\lambda_r(M_n) = 2\cos(\frac{r\pi}{n}) + (-1)^r \quad r = 1, \ldots, 2n.$$

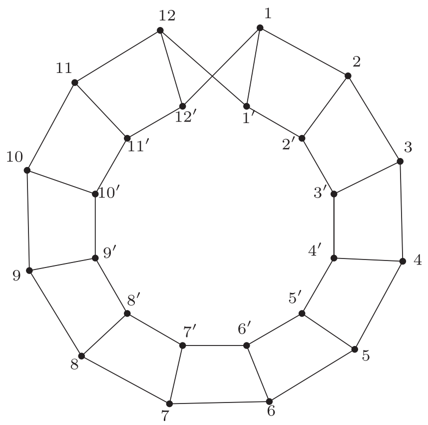

Figure 2: The Mӧbius Ladder M_{12}

Corollary 3.5. *The Laplacian revised Szeged eigenvalues of the Möbius ladder M_n are given by*

$$\mu_r^{'}(M_n) = n^2[3 - (-1)^r - 2\cos(\frac{r\pi}{n})],$$

for $r = 1, \ldots, 2n$.

Proof. Apply Proposition 3.3. ☐

Our third example of this section is about strongly regular graphs. A strongly regular graph with parameters (n, k, a, c) is a simple $n-$vertex graph which is $k-$regular, $k \neq 0, n-1$, any two adjacent vertices have exactly a common neighbours and two non-djacent vertices have exactly c common neighbours. A strongly regular graph is called primitive if both G and its complement are connected. It is well-known in a primitive strongly regular graph $c \neq 0$ and $c \neq k$.

Proposition 3.6. *Let G be a primitive strongly regular graph with parameters (n,k,a,c). Then $Sz^*M(G) = \frac{n^2}{4}A(G)$ and $LSz^*M(G) = \frac{n^2}{4}L(G)$. Hence, $\sigma_r(G) = \frac{n^2}{4}\lambda_r(G)$ and $\mu_r^{'}(G) = \frac{n^2}{4}\mu_r(G)$.*

Proof. The proof is similar to [4, Proposition 4] and so omitted. □

3.2. Graph operations

Suppose that G_1 and G_2 are two graphs. Their Cartesian product $G_1 \square G_2$ is a graph on the vertex set $V(G_1) \times V(G_2)$ and the vertices (u_1, u_2) and (v_1, v_2) are adjacent in $V(G_1) \times V(G_2)$ if and only if either $(u_1 = v_1$ and $u_2 v_2 \in E(G_2))$ or $(u_1 v_1 \in E(G_1)$ and $u_2 = v_2)$. The adjacency matrix of $G_1 \square G_2$ is given by

$$A(G_1 \square G_2) = I_{n_1} \otimes A(G_2) + A(G_1) \otimes I_{n_2},$$

where n_1 and n_2 are the number of vertices of G_1 and G_2, respectively, and $A \otimes B$ is the tensor product of matrices A and B [2, p. 430]. The Laplacian matrix of $G_1 \square G_2$ is given by analogous formula

$$L(G_1 \square G_2) = I_{n_1} \otimes L(G_2) + L(G_1) \otimes I_{n_2}.$$

Suppose the eigenvalues of G_1 are denoted by λ_{1r}, $1 \leq r \leq n_1$, and the eigenvalues of G_2 by λ_{2s}, $1 \leq s \leq n_2$. Then the eigenvalues of $G_1 \square G_2$ are given by

$$\lambda_{r,s}(G_1 \square G_2) = \lambda_{1r}(G_1) + \lambda_{2s}(G_2),$$

where $1 \leq r \leq n_1$ and $1 \leq s \leq n_2$ [2, Chapter 2]. Therefore,

Proposition 3.7. *Suppose that G_1 and G_2 are two connected graphs on n_1 and n_2 vertices, respectively. Then*

$$Sz^*M(G_1 \square G_2) = n_2^2 Sz^*M(G_1) \otimes I_{n_2} + n_1^2 I_{n_1} \otimes Sz^*M(G_2).$$

Proof. A similar argument like as [4, Theorem 5] shows that each shortest path in $G_1 \square G_2$ from vertex (u_1, z) to (u_1, v_2) in $G_1 \times G_2$ must contain either the edge $(u_1, u_2)(u_1, v_2)$, or any of n_1 edges parallel to it in $G_1 \square G_2$. Hence $n_{(u_1,u_2)}((u_1,u_2)(u_1,v_2)) = n_1 n_{u_2}(u_2, v_2)$. In the same way, we have $n_{(u_1,v_2)}((u_1,u_2)(u_1,v_2)) = n_1 n_{v_2}(u_2, v_2)$. Finally, for the equal distance vertices to both end vertices we have $n_0((u_1,u_2)(u_1,v_2)) = n_1 n_0(u_2, v_2)$. Thus, the revised Szeged matrix of $G_1 \square G_2$ is $Sz^*M(G_1 \square G_2) = n_2^2 Sz^*M(G_1) \otimes I_{n_2} + n_1^2 I_{n_1} \otimes Sz^*M(G_2)$. The Laplacian revised Szeged matrix of $G_1 \square G_2$ has the same form. This completes the proof. □

Proposition 3.8. *The revised Szeged eigenvalues of $G_1 \Box G_2$ are given by*

$$\sigma_{r,s}(G_1 \Box G_2) = n_2^2 \sigma_r(G_1) + n_1^2 \sigma_s(G_2)$$

and the Laplacian revised Szeged eigenvalues of $G_1 \Box G_2$ are given by

$$\mu'_{r,s}(G_1 \Box G_2) = n_2^2 \mu'_r(G_1) + n_1^2 \mu'_s(G_2)$$

for $r = 1, \ldots, n_1$, $s = 1, \ldots, n_2$.

As an application of Proposition 3.8, we can calculate the revised Szeged eigenvalues of C_4-nanotorus $C_m \Box C_n$. The revised Szeged and Laplacian revised Szeged eigenvalues are as follows:

(i) $\sigma_{r,s}(C_m \Box C_n) = \frac{n^2 m^2}{4}[\cos(\frac{2r\pi}{m}) + \cos(\frac{2s\pi}{n})]$,
(ii) $\mu'_{r,s}(C_m \Box C_n) = \frac{n^2 m^2}{4}[2 + \sin^2(\frac{r\pi}{m}) + \sin^2(\frac{s\pi}{n})]$,

for $r = 1, \ldots, m$, $s = 1, \ldots, n$.

Using an inductive argument, we can generalize Proposition 3.8 to an arbitrary number of graphs. Suppose $G_1, \ldots, G_s$ are graphs and $n_i = |V(G_i)|$, $1 \le i \le s$.

Proposition 3.9. *The revised Szeged and the Laplacian revised Szeged eigenvalues of $G = \prod_{i=1}^{s} G_i$ are*

$$\sigma_{i_1,\ldots,i_s}(G) = (\prod_{i=1}^{s} n_i^2)(\sum_{k=1}^{s} \frac{\sigma_{i_k}(G_k)}{n_k^2}) \quad 1 \le i_k \le n_k$$

and

$$\mu'_{i_1,\ldots,i_s}(G) = (\prod_{i=1}^{s} n_i^2)(\sum_{k=1}^{s} \frac{\mu'_{i_k}(G_k)}{n_k^2}) \qquad 1 \le i_k \le n_k,$$

respectively.

The above formulas can be simplified for Cartesian powers as follows:

Corollary 3.10. *For a connected graph G,*

(i) $\sigma_{i_1,\ldots,i_s}(G^s) = n^{2(s-1)}(\sum_{k=1}^{s} \sigma_{i_k}(G)) \qquad 1 \le i_k \le n_k,$

(ii) $\mu'_{i_1,\ldots,i_s}(G^s) = n^{2(s-1)}(\sum_{k=1}^{s} \mu'_{i_k}(G)) \qquad 1 \le i_k \le n_k.$

A hypercube Q_n is defined as the Cartesian power of n copies of K_2. By Corollary 3.7, $\sigma_r(Q_n) = 4^{n-1}(n-2r)$ with multiplicity $\binom{n}{r}$, where $0 \le r \le n$ and $\mu'_r(Q_n) = 4^{n-1}(2n-2r)$ with multiplicity $\binom{n}{r}$ for $r = 0, \dots, n$.

We assume that $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are two graphs. Then the lexicographic product of G_1 and G_2, $G_1[G_2]$, is a graph that $V(G_1[G_2]) = V_1 \times V_2$ and two vertices (u_1, v_1) and (u_2, v_2) in $G_1[G_2]$ are adjacent if and only if either $u_1u_2 \in E(G_1)$ or $u_1 = u_2$ and $v_1v_2 \in E(H)$. Let $A(G_1)$ and $A(G_2)$ be adjacency matrices of G_1 and G_2, respectively. We also assume that I_{n_1} denotes the identity matrix of order n_1 and J_{n_2} be the all 1 matrix of order n_2. Then the adjacency matrix of $A(G_1[G_2])$ is equal to $A(G_1) \otimes J_{n_2} + I_{n_1} \otimes A(G_2)$.

Proposition 3.11. *Suppose that G_1 is a graph with n_1 vertices and G_2 is a k-regular graph with n_2 vertices. Then $Sz^*M(G_1[G_2]) = n_2^2 Sz^*M(G_1) \otimes J_{n_2} + \frac{n_1^2 n_2^2}{4} I_{n_1} \otimes A(G_2)$.*

Proof. Let $e_1 = ((a,x)(b,y)) \in E(G_1[G_2])$ such that $ab \in E(G_1)$. So, $n_1(e_1) = (n_1(ab)-1)|G_2| + |G_2| - \deg_{G_2}(y) - 1$ and $n_2(e_1) = (n_2(ab)-1)|G_2| + |G_2| - \deg_{G_2}(x) - 1$ and $n_0(e_1) = (n_0(ab)-1)|G_2| + \deg_{G_2}(x) + \deg_{G_2}(y) + 2$. Since G_2 is k-regular then $Sz^*(e_1) = (n_1(e_1) + n_0(e_1)/2)(n_2(e_1) + n_0(e_1)/2)$ and by a simple calculation we have $Sz^*(e_1) = |G_2|^2 Sz^*(ab)$. Let $e_1 = ((a,x)(a,y)) \in E(G_1[G_2])$ such that $xy \in E(G_2)$. Then we get $n_1(e_2) = \deg_{G_2}(x) - N(xy)$, $n_2(e_2) = \deg_{G_2}(y) - N(xy)$ and $n_0(e_2) = (|G|-1)|G_2| + |G_2| - 2(k - N(xy))$, where $N(xy) = \{w \in V(G_2) | d(x,w) = d(w,y) = 1\}$. Thus, $Sz^*(e_2) = \frac{(|G_1||G_2|)^2}{4}$ and so

$$Sz^*M(G_1[G_2]) = n_2^2 Sz^*M(G_1) \otimes J_{n_2} + \frac{n_1^2 n_2^2}{4} I_{n_1} \otimes A(G_2).$$

Hence the result. □

Corollary 3.12. *Suppose G_1 is a graph with n_1 vertices and G_2 is a k-regular distance-balanced graph with n_2 vertices. Then*

$$Sz^*M(G_1[G_2]) = n_2^2 Sz^*M(G_1) \otimes J_{n_2} + n_1^2 I_{n_1} \otimes Sz^*M(G_2).$$

The corona product or simply corona of G_1 and G_2 is defined as the disjoint union of one copy of G_1 and $|V_1|$ copies of G_2 in such a way that the $i-th$ vertex of G_1 is connected to all vertices of the $i-th$ copy of G_2. This graph is denoted by $G_1 \circ G_2$. One can see that $G_1 \circ G_2$ has $n_1(n_2+1)$ vertices and $m_1 + n_1(n_2 + m_2)$ edges, where $n_i = |V(G_i)|$ and $m_i = |E(G_i)|$, $i = 1,2$.

Proposition 3.13. *Suppose that G_1 and G_2 are two graphs, $n_i = |V(G_i)|$ and $m_i = |E(G_i)|$, $i = 1,2$. Then*

$$\begin{aligned} Sz^*(G_1 \circ G_2) = {} & (n_2+1)Sz^*(G_1) + n_1^3(n_2+1) - (n_1(n_2+1)-2)m_2 \\ & -\frac{n_1}{4} \sum_{v \in V(G_2)} \deg^2(v) + \frac{n_1^2(n_2+1)^2 m_2}{4} - \sum_{e=vw \in E(G_2)} (\deg v - \deg w)^2. \end{aligned}$$

Proof. We have three types of edges in $G_1 \circ G_2$, the edges of G_1, the edges between vertices of G_1 and vertices of the corresponding copy of G_2 and the edges of copies of G_2. We first assume that $uv = e_1 \in G_1$. Then,

$$\begin{aligned} n_0(e_1|G_1 \circ G_2) &= n_0(e_1|G_1)(|V(G_2)|+1) = (n_2+1)n_0(e_1|G_1),\\ n_u(e_1|G_1 \circ G_2) &= n_u(e_1|G_1)(|V(G_2)|+1) = (n_2+1)n_u(e_1|G_1),\\ n_v(e_1|G_1 \circ G_2) &= n_v(e_1|G_1)(|V(G_2)|+1) = (n_2+1)n_v(e_1|G_1). \end{aligned}$$

So, $Sz^*(e_1|G_1 \circ G_2) = (|V(G_2)+1)Sz^*(e_1|G_1) = (n_2+1)Sz^*(e_1|G_1)$. Notice that the number of these edges is m_1. Next we assume that $e_2 = uv$ such that $u \in V(G_1)$ and $v \in V(G_2)$. Then $n_0(e_2|G_1 \circ G_2) = \deg(v|G_2)$, $n_u(e_2|G_1 \circ G_2) = (|V(G_1)|-1)(|V(G_2)|+1) + |V(G_2)| - \deg(v|G_2) = n_1n_2 + n_1 - 1 - \deg(v|G_2)$ and $n_v(e_1|G_1 \circ G_2) = 1$. So,

$$Sz^*(e_2|G_1 \circ G_2) = n_1n_2 + n_1 - 1 - 1/2(n_1n_2 + n_1 - 2)\deg(v|G_2) - 1/4\deg^2(v|G_2)).$$

We note that the number of such edges is n_1n_2. Finally, we assume that $e_3 = vw \in E(G_2)$. Then,

$$\begin{aligned} n_v(vw|G_1 \circ G_2) &= \deg(v|G_2) - 1,\\ n_w(vw|G_1 \circ G_2) &= \deg(w|G_2) - 1,\\ n_0(vw|G_1 \circ G_2) &= |V(G_1)||V(G_2)| + |V(G_1)| - \deg(v|G_2) - \deg(w|G_2) + 2,\\ &= n_1n_2 + n_1 + 2 - (\deg(v|G_2) + \deg(w|G_2)). \end{aligned}$$

So, $Sz^*(e_3) = \frac{1}{4}((n_1n_2 + n_1)^2 - (\deg(v|G_2) - \deg(w|G_2))^2)$ and the number of these edges is n_1m_2. Therefore,

$$\begin{aligned} Sz^*(G_1 \circ G_2) &= \sum_{e_1} Sz^*(e_1) + \sum_{e_2} Sz^*(e_2) + \sum_{e_3} Sz^*(e_3)\\ &\quad + n_1 \sum_{v \in V(G_2)} (n_1n_2 + n_1 - \frac{1}{2}(n_1n_2 + n_1 - 2)\deg(v|G_2) - \frac{1}{4}\deg^2(v|G_2))\\ &\quad + \sum_{e_3 = vw \in G_2} [1/4(n_1n_2 + n_1)^2 - (\deg(v|G_2) - \deg(w|G_2))^2]\\ &= (n_2+1)Sz^*(G_1) + n_1^3(n_2+1) - (n_1(n_2+1) - 2)m_2 + (n_2+1)Sz^*(G_1)\\ &\quad - \frac{n_1}{4} \sum_{v \in V(G_2)} \deg^2(v) + \frac{n_1^2(n_2+1)^2 m_2}{4} - \sum_{e = vw \in E(G_2)} (\deg v - \deg w)^2. \end{aligned}$$

This completes the proof. $\square$

3.3. Bounds on the revised szeged spectrum

We are now analyzing the revised Szeged spectra of general graphs. Our first result in this section depends on well-known result in algebraic graph theory which states that if G is a connected graph with n vertices, m edges, t triangles, q qaudrangles and $\chi(G,x) = x^n + c_1x^{n-1}+c_2x^{n-2}+c_3x^{n-3}+c_4x^{n-4}+\cdots+c_n$ is its characteristic polynomial, then $c_1 = 0$, $-c_2 = m$, $-c_3 = 2t$ and $c_4 = 2q$ [1, Corollary 2.3].

Lemma 3.14. *Suppose G is a connected graph. Then, $tr(A^4) = 8q + M_1(G) - tr(A^2)$, where $tr(X)$ denotes the trace of a matrix X, $M_1(G)$ is the first Zagreb index of G and Sq the number of quadrangles in G.*

Using those interpretations we can deduce bounds on the second, third and fourth revised Szeged spectral moment of a graph G.

Proposition 3.15. *Let G be a connected graph on n vertices and $\sigma_i, 1 \leq i \leq n$, be its revised Szeged eigenvalues. Then*

1. $2(n-1)^2m \leq \sum_{i=1}^{n} \sigma_i^2 \leq \frac{n^4}{8}m,$
2. $6(n-1)^3t \leq \sum_{i=1}^{n} \sigma_i^3 \leq 6(\frac{n^2}{4})^3t,$
3. $(n-1)^4[8q+M_1(G)-2(n-1)^2m] \leq \sum_{i=1}^{n} \sigma_i^4 \leq (\frac{n^2}{4})^4[8q+M_1(G)-2(n-1)^2m].$

The left inequality in (1) holds if and only if $G = S_n$, the $n-$vertex star graph, and the right equality satisfies if and only if G is distance−balanced.

Proof. To prove (1) we denote the elements of the k-th power of $Sz^*M(G)$ by $s^{(k)}(i,j)$. Since $(n-1)^k a_{ij}^{(k)} \leq s_{ij}^{(k)} \leq (\frac{n^2}{4})^k a_{ij}^{(k)}$ and $\sigma_1^2+\ldots+\sigma_n^2 = tr(Sz^*M(G)^2)$,

$$2(n-1)^2m = \sum_{i=1}^{n}(n-1)^2a_{ii}^{(2)} \leq \sum_{i=1}^{n}\sigma_i^2 = \sum_{i=1}^{n}s_{ii}^{(2)} \leq \sum_{i=1}^{n}(\frac{n^2}{4})^2a_{ii}^{(2)} = \frac{n^4}{16}\times 2m = m\frac{n^4}{8}.$$

The left equality holds if and only if for each $e = uv \in E(G)$, $\{n_u(e), n_v(e)\} = \{n-1,1\}$, $n_0(e) = 0$. But this can be happened when $G \cong S_n$.

Let us assume that t_i denotes the number of triangles containing the vertex v_i. Since $tr(Sz^*M(G)^3) = \sum_{i=1}^{n}\sigma_i^3$, $(n-1)^3t_i = a_{i,i}^{(3)} \leq s_{i,j}^{(3)} \leq (\frac{n^2}{4})^3a_{i,i}^{(3)}$. This implies that

$$(n-1)^3\sum_{i=1}^{n}t_i \leq \sum_{i=1}^{n}s_{i,j}^{(3)} \leq \sum_{i=1}^{n}\sigma_i^{(3)} \leq (\frac{n^2}{4})^3\sum_{i=1}^{n}a_{i,i}^{(3)} = (\frac{n^2}{4})^3\times 6t.$$

Thus, $6t(n-1)^3 \leq \sum_{i=1}^{n} \sigma_i^{(3)} \leq 6(\frac{n^2}{4})^3 t$. The last part is similar to parts 1 and 2 and so omitted. □

The spectral radius of a square matrix A is the supremum among the absolute values of the elements in the spectrum of A, which is denoted by $\rho(A)$ [5, p. 177]. The revised Szeged spectral radius $\rho^*(G)$ is defined as the spectral radius of matrix $Sz^*M(G)$.

Proposition 3.16. *Let G be a connected graph on n vertices. Then $\rho^*(G) \leq \frac{n^2}{4}\Delta(G)$, where $\Delta(G)$ denotes the maximum degree of all vertices in G. Moreover, equality holds if and only if G is regular and distance balanced.*

Proof. Let $\mathbf{x} = [x_1, \ldots, x_n]^T$ be the eigenvector of $Sz^*M(G)$ corresponding to the eigenvalue σ. If $|x_m| = \max\{|x_1|, \ldots, |x_n|\}$, then $\sum_{j=1}^{n} s_{m,j}x_j = \sigma x_m$. Therefore, $|\sigma||x_m| \leq \sum_{j=1}^{n} s_{m,j}|x_j| \leq \frac{n^2}{4}\Delta(G)|x_m|$ and hence $|\sigma| \leq \frac{n^2}{4}\Delta(G)$. Clearly, the equality holds if and only if G is regular and distance balanced. □

Proposition 3.17. *Let G be a connected graph on n vertices and m edges. Then*

$$\frac{2}{m}Sz^*(G)^2 \leq \sum_{i=1}^{n} \sigma_i^2 \leq \min\{\frac{n^2}{2}Sz^*(G), 2Sz^*(G)^2 - 2m(m-1)(n-1)^2\}$$

The left(right) equality holds if and only if $G = K_2$.

Proof. Suppose that $S = \sum_{i=1}^{n} \sigma_i^2$. It is enough to prove that $S \leq \frac{n^2}{2}Sz^*(G)$, $S \leq 2Sz^*(G)^2 - 2m(m-1)(n-1)^2$ and $\sqrt{S} \geq \sqrt{\frac{2}{m}}Sz^*(G)$. Clearly, $S = (\sum_{i=1}^{n} \sigma_i)^2 - 2\sum_{i<j} \sigma_i\sigma_j$ and then $C_2 = \sum_{i<j} \sigma_i\sigma_j$. Furthermore, $S = 2\sum_{i<j}(n_{v_i} + n_0/2)^2(n_{v_j} + n_0/2)^2$ and since $(n-1) \leq (n_{v_i} + n_0/2)(n_{v_j} + n_0/2) \leq \frac{n^2}{4}$,

$$\begin{aligned}
S &= 2\sum_{i<j}((n_{v_i} + \frac{n_0(e)}{2})(n_{v_j} + \frac{n_0(e)}{2}))^2 \\
&= 2\Big[\sum_{i<j}((n_{v_i} + \frac{n_0(e)}{2})(n_{v_j} + \frac{n_0(e)}{2}))^2 \\
&\quad -2\sum_{uv \neq xy}(n_u + \frac{n_0(uv)}{2})(n_v + \frac{n_0(uv)}{2})(n_x + \frac{n_0(xy)}{2})(n_y + \frac{n_0(xy)}{2})\Big] \\
&\leq 2Sz^*(G)^2 - 2m(m-1)(n-1)^2.
\end{aligned}$$

Now, the equality holds if and only if $G = S_n$. The second inequality follows from the Cauchy-Schwarz inequality as:

$$\begin{aligned}
Sz^*(G) &= \sum_{e=uv\in E(G)}(n_u + \frac{n_0(uv)}{2})(n_v + \frac{n_0(uv)}{2}) \\
&\leq \sqrt{m\sum_{e=uv\in E(G)}((n_u + \frac{n_0(uv)}{2})(n_v + \frac{n_0(uv)}{2}))^2} = \sqrt{\frac{m}{2}S}.
\end{aligned}$$

Hence the result. □

Acknowledgements

The authors are indebted to anonymous referee for his/her suggestions and helpful remarks. The research of the second author is partially supported by the University of Kashan under grant no 364988/2.

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