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Research Article

Complexity of the Szeged index, edge orbits, and some nanotubical fullerenes

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Abstract

Let I be a summation-type topological index. The I-complexity $C_I(G)$ of a graph G is the number of different contributions to $I(G)$ in its summation formula. In this paper the complexity $C_{\rm Sz}(G)$ is investigated, where Sz is the well-studied Szeged index. Let $O_e(G)$ (resp. $O_v(G)$) be the number of edge (resp. vertex) orbits of G. While $C_{\rm Sz}(G) \le O_e(G)$ holds for any graph G, it is shown that for any $m \ge 1$ there exists a vertex-transitive graph G_m with $C_{\rm Sz}(G_m) = O_e(G_m) = m$. Also, for any $1 \le k \le m+1$ there exists a graph $G_{m,k}$ with $C_{\rm Sz}(G_{m,k}) = O_e(G_{m,k}) = m$ and $C_W(G_{m,k}) = O_v(G_{m,k}) = k$. The Sz-complexity is determined for a family of (5,0)-nanotubical fullerenes and the Szeged index is compared with the total eccentricity.

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1. Introduction

In mathematical chemistry, any function which assigns a real number to a (chemical) graph and is invariant under graph isomorphism is called a *topological index*. Of course, one has countless possibilities how to define a (new) topological index; hence it is important to design it to be applicable and, also not negligible, mathematically appealing. The reader is invited to books [16, 17, 31] for examples of topological indices that have passed these requirements. We also refer to [13, 28] for a couple of recent chemical applications, to [7] for a recent investigation of several infinite convex benzenoid networks via numerous topological indices, as well as to [19] for studies of additional topological indices on hex-derived networks.

In this paper we are primarily interested in the Szeged index that turned out to be one of the relevant topological indices. It was introduced in [15] and proved to be chemically relevant in [8,20] as well as in [7], where Szeged-like indices are involved in the investigation. The papers [18, 25] present a couple of recent developments on the Szeged index.

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Let $G = (V(G), E(G))$ be a graph. Suppose that a topological index I either of the form

$$I(G) = \sum_{v \in V(G)} f(v)\,, \tag{1.1}$$

or of the form

$$I(G) = \sum_{e \in E(G)} f(e)\,, \tag{1.2}$$

where $f : V(G) \to \mathbb{R}$ (resp. $f : E(G) \to \mathbb{R}$) is a real function. The most striking example is obtained by setting $f(v)$ to be the sum of the distances from v to all the other vertices, because in this case (1.1) reads as $I(G) = 2W(G)$, where $W(G)$ is the Wiener index of G. Vertices u and u' (resp. edges e and e') are in relation $\sim_I$ if $f(u) = f(u')$ (resp. $f(e) = f(e')$). Clearly, $\sim_I$ is an equivalence relation. Let $V(G)/_{\sim_I} = \{V_1, \ldots, V_k\}$ (resp. $E(G)/_{\sim_I} = \{E_1, \ldots, E_k\}$) be its equivalence classes and let $v_i \in V_i$ (resp. $e_i \in E_i$) for $i \in [k] = \{1, \ldots, k\}$. Then (1.1) can be rewritten as

$$I(G) = \sum_{i=1}^{k} |V_i| f(v_i)\,, \tag{1.3}$$

while (1.2) reduces to

$$I(G) = \sum_{i=1}^{k} |E_i| f(e_i)\,. \tag{1.4}$$

The value k is called the *I-complexity* of G and denoted $C_I(G)$. This concept was introduced in [4] and studied on the connective eccentricity index; see [14, 32] for more information on the latter index. Earlier, the complexity with respect to the Wiener index was investigated in [3] under the name Wiener dimension. For recent developments on the Wiener complexity see [1,5,21]. In addition, in [2] the Szeged and the PI_v dimension was investigated.

The paper is organized as follows. In the next section additional concepts needed are introduced. In the central part of the paper, Section 3, the Sz-complexity of graphs is compared to the numbers of their edge orbits O_e and the number of their vertex orbits O_v. It is observed that for any graph G, $C_{\rm Sz}(G) \le O_e(G)$, and demonstrated that for any integer $m \ge 1$ there exists a vertex-transitive graph G_m with $C_{\rm Sz}(G_m) = O_e(G_m) = m$. Moreover, for any $1 \le k \le m+1$ there exists a graph $G_{m,k}$ with $C_{\rm Sz}(G_{m,k}) = O_e(G_{m,k}) = m$ and $C_W(G_{m,k}) = O_v(G_{m,k}) = k$. In Section 4 the Sz-complexity is determined for a family of (5,0)-nanotubical fullerenes. As a consequence the Szeged index of these fullerenes is determined. In the final section it is proved that if G is a connected graph of order at least 4, then ${\rm Sz}(G) \ge {\rm Ecc}(G)$, where equality holds if and only if $G = P_4$.

2. Preliminaries

All graphs considered in this paper are connected. The *degree* of a vertex u of a graph G is denoted with $\deg_G(u)$. The *distance* between vertices u and v of a graph G is denoted by $d_G(u, v)$. The *distance $d_G(v)$ of vertex v* is defined as $d_G(v) = \sum_{u \in V(G)} d_G(v, u)$. The *eccentricity* ${\rm ecc}_G(v)$ of v is the largest distance between v and the vertices of G. Whenever G is clear form the context, we may omit the index G in the above notation. The maximum and the minimum eccentricity among all vertices of G are the *diameter* ${\rm diam}(G)$ and the *radius* ${\rm rad}(G)$, respectively.

The *Wiener index* of graph G is the sum of distances between all pairs of vertices of G, that is,

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} d(v)\,.$$

Let $e = uv$ be an edge of graph G. The number of vertices of G lying closer to u than to v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G lying closer to v than to u. The *Szeged index* [15] of G is defined with

$$\mathrm{Sz}(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e)\,.$$

The *total eccentricity* of G is defined as

$$\mathrm{Ecc}(G) = \sum_{v\in V(G)} \mathrm{ecc}(v)\,.$$

Let $\mathrm{Aut}(G)$ denote the automorphism group of G. A graph G is *vertex-transitive* if two any vertices u and v of G there exists $\alpha \in \mathrm{Aut}(G)$ such that $\alpha(u) = v$. Let $O_v(G)$ and $O_e(G)$ be the number of vertex orbits and edge orbits of G under the action of $\mathrm{Aut}(G)$, respectively. A function $f : V(G) \to \mathbb{R}$ (resp. $f : E(G) \to \mathbb{R}$) is a *graph function* if it is invariant under automorphisms of G; that is, if $\alpha \in \mathrm{Aut}(G)$ and u and u' belong to the same vertex orbit (resp. e and e' belong to the same edge orbit), then $f(u) = f(u')$ (resp. $f(e) = f(e')$).

We will use the following result that goes back to [12].

Proposition 2.1. *If $e = uv$ is an edge of a connected graph G, then $d_G(u) - d_G(v) = n_v(e) - n_u(e)$.*

3. Sz-complexity versus number of edge orbits

Suppose that a topological index I is of the form (1.1) or (1.2), where f is a graph function. Then by definition,

$$C_I(G) \le O_v(G) \quad (\text{resp. } C_I(G) \le O_e(G))\,. \tag{3.1}$$

We note in passing that if $C_I(G) \le O_v(G)$, then $C_I(G) \le O_e(G) + 1$. This follows from a result of Buset [9] asserting that if G is a (connected) graph, then $O_v(G) \le O_e(G) + 1$.

Theorem 3.1. *If G is a graph, then $C_{\mathrm{Sz}}(G) \le O_e(G)$. Moreover, for any integer $m \ge 1$ there exists a vertex-transitive graph G_m with $C_{\mathrm{Sz}}(G_m) = O_e(G_m) = m$.*

Proof. For the first assertion, in view of (3.1) it suffices to prove that the function $f(e) = n_u(e)n_v(e)$, where $e = uv \in E(G)$, is a graph function. Hence let $e = uv$ and $e' = xy$ be edges from the same edge orbit, and let $\alpha \in \mathrm{Aut}(G)$ such that $\alpha(u) = x$ and $\alpha(v) = y$. Let $\Gamma_k(u) = \{w \in V(G) \mid d(u,w) = k\}$, $0 \le k \le \mathrm{ecc}(u)$. We claim that $n_u(e) = n_x(e')$ and $n_v(e) = n_y(e')$. For this sake observe first that $n_u(uv) = \sum_{k=0}^{\mathrm{ecc}(u)} |\Gamma_k(u) \bigcap \Gamma_{k+1}(v)|$. Furthermore,

$$w \in \Gamma_k(u) \bigcap \Gamma_{k+1}(v) \Leftrightarrow \alpha(w) \in \Gamma_k(\alpha(u)) \bigcap \Gamma_{k+1}(\alpha(v)) = \Gamma_k(x) \bigcap \Gamma_{k+1}(y).$$

Therefore

$$n_u(uv) = \sum_{k=0}^{\mathrm{ecc}(u)} |\Gamma_k(u) \bigcap \Gamma_{k+1}(v)| = \sum_{k=0}^{\mathrm{ecc}(x)} |\Gamma_k(x) \bigcap \Gamma_{k+1}(y)| = n_x(xy)\,.$$

This proves the first assertion of the theorem.

Let $m \ge 1$ and set $n = 3m + 1$. Define the graph G_m on the vertex set $[n]_0 = \{0, 1, \ldots, n-1\}$, where the vertex i is adjacent to vertices $i\pm1, \ldots, i\pm m \pmod n$. Clearly, G_m is vertex-transitive. (Alternatively, G_m belongs to the family of circulant graphs which are well-known to be vertex-transitive.) Consider now the edge ij, where $j = i \pm k$, $1 \le k \le m$. Then ij lies in precisely $m - k + 1$ complete subgraphs K_{m+1}. It follows that G_m contains at least m edge orbits. On the other hand, any two edges that differ by the same integer, are in the same edge orbit. We conclude that $O_e(G_m) = m$. Finally, any pair of vertices has a common adjacent vertex, hence $\mathrm{diam}(G_m) = 2$. Moreover, since G_m

is $(2m)$-regular, vertices i and $j = i \pm k$, $1 \leq k \leq m$, have exactly $2m-k-1$ common adjacent vertices. Consequently $n_i(ij) = n_j(ij) = k+1$. Therefore, $C_{\rm Sz}(G_m) = m$. □

In view of (3.1) the reader might wonder why the first assertion of Theorem 3.1 requires a proof. To see that the assertion need not be true in general, consider the following example. Let G be a graph with the vertex set $[n]_0$, and define the invariant $\mathrm{Sz}'(G) = \sum_{e=ij\in E(G)} (n_i(e) - n_j(e))$. Then in general $C_{\mathrm{Sz}'}(G) \leq O_e(G)$ does not hold. For a small example consider the path P_3 of order 3. Clearly, $O_e(P_3) = 1$, but $C_{\mathrm{Sz}'}(P_3) = 2$.

In Theorem 3.1 we have seen that there exist graphs with a single vertex orbit and with an arbitrary large Sz-complexity. On the other hand, we also have:

Proposition 3.2. *There exists an infinite family of non edge-transitive graphs with Sz-complexity equal to* 1*.*

Proof. Let W_n, $n \geq 3$, be the n-wheel, that is, the graph obtained from the n-cycle C_n and an extra vertex joined to all the vertices of the cycle. The cogwheel M_n is then obtained from W_n by subdividing each edge of C_n by one vertex. Clearly, M_n is not edge-transitive. On the other hand it is straightforward to infer that for any edge $e = uv \in E(M_n)$ we have $\{n_u(e), n_v(e)\} = \{3, 2n-2\}$, so that $C_{\rm Sz}(M_n) = 1$. □

It is straightforward to see that the cogwheel M_n has two edge orbits. Hence an interesting question appears whether there exist (infinite families of) graphs with Sz-complexity equal to 1 and with an arbitrary number of edge orbits.

By the above-mentioned Buset's result [9] we have $O_v(G) \leq O_e(G) + 1$. We next show that comparing the Sz-complexity with the W-complexity anything else can happen. More precisely:

Theorem 3.3. *If $m \geq 1$ and $1 \leq k \leq m+1$, then there exists a graph $G_{m,k}$ with $C_{\rm Sz}(G_{m,k}) = O_e(G_{m,k}) = m$ and $C_W(G_{m,k}) = O_v(G_{m,k}) = k$.*

Proof. Let $m \geq 1$ and set $G_{m,m+1} = P_{2m+1}$. Then it can be routinely checked that $C_{\rm Sz}(G_{m,m+1}) = O_e(G_{m,m+1}) = m$ and $C_W(G_{m,m+1}) = O_v(G_{m,m+1}) = m+1$.

Suppose in the rest that $m \geq 1$ and $1 \leq k \leq m$. Let G_m be the graph of order $3m+1$ as constructed in the proof of Theorem 3.1, where $V(G_m) = [3m+1]_0$. Let $G_{m,k}$ be the graph obtained from a disjoint union of G_{m-k+1} and $m-k+1$ copies of the path P_k, by identifying each of the vertices of G_{m-k+1} with an end-vertex of a respective copy of P_k. The construction is illustrated in Fig. 1 with the graph $G_{5,4}$. Note also that $G_{m,1} = G_m$.

As already inferred in the proof of Theorem 3.1, $O_e(G_{m-k+1}) = m-k+1$. This in turn implies that $O_e(G_{m,k}) = (m-k+1) + (k-1) = m$. Consider now the edges $0j$, $j \in [m-k+1]$, of G_{m-k+1} (considered as a subgraph of $G_{m,k}$), and observe that $a_j = n_0(0j) = n_j(0j) = (j+1)k$. Furthermore, for the $k-1$ edges e_i of an arbitrary fixed attached P_k, we easily infer that their contributions to the Szeged index are $b_i = i(3k(m-k+1)+k-i)$, $i \in [k-1]$, because $|V(G_{m,k})| = 3k(m-k+1)+k$. Since for any $i \in [k-1]$ and any $j \in [m-k+1]$ we have $i(3k(m-k+1)+k-i) > (j+1)k$, there exist $(m-k+1)+(k-1) = m$ different contributions to $\mathrm{Sz}(G_{m,k})$. Hence in view of the second assertion of (3.1) and the above fact that $O_e(G_{m,k}) = m$ we conclude that $C_{\rm Sz}(G_{m,k}) = m$.

Since G_{m-k+1} is vertex-transitive, it follows directly that $O_v(G_{m,k}) = k$. Moreover, by symmetry, all the vertices of G_{m-k+1} (considered as vertices of $G_{m,k}$) have the same distance in $G_{m,k}$. Consider now the vertices of an arbitrary fixed P_k subgraph of $G_{m,k}$. Then by iterative applications of Proposition 2.1 we get that all these k vertices have different distances. Hence by the first assertion of (3.1) we conclude that $C_W(G_{m,k}) = k$. □

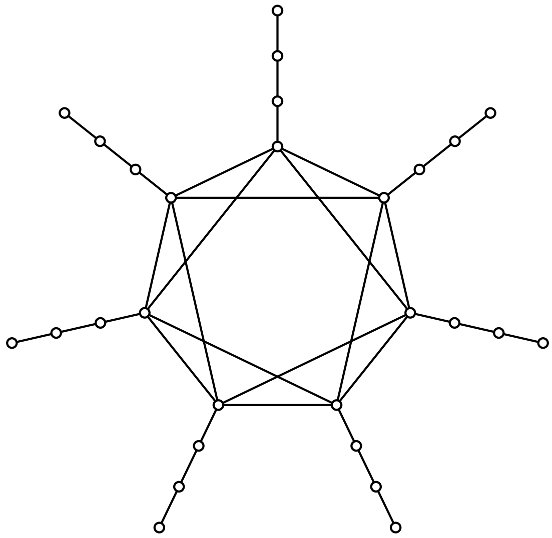

Figure 1. The graph $G_{5,4}$

Considering the graphs from the proof of Theorem 3.3 and noting that $C_{\mathrm{Ecc}}(P_{2m+1}) = m+1$ for $m \geq 1$ and that $C_{\mathrm{Ecc}}(G_{m,k}) = k$ for $m \geq 1$ and $1 \leq k \leq m$, we get in passing the following result.

Corollary 3.4. *If $m \geq 1$ and $1 \leq k \leq m+1$, then there exists a graph $G_{m,k}$ with $C_{\mathrm{Sz}}(G_{m,k}) = O_e(G_{m,k}) = m$ and $C_{\mathrm{Ecc}}(G_{m,k}) = O_v(G_{m,k}) = k$.*

4. Sz-complexity of the fullerenes C_{10n}

In this section we compute the Sz-complexity of a family of fullerene graphs. This yields another infinite family of (chemical) graphs for which the Sz-complexity coincides with the number of edge orbits.

A fullerene graph is a 3-connected, 3-regular plane graph with only pentagonal and hexagonal faces. They have exactly twelve pentagonal faces. Here we consider the family of fullerenes C_{10n}, $n \geq 2$, known as (5,0)-nanotubical fullerenes. (For distance properties of C_{10n} see [3,6].) The fullerene C_{10n} contains $10n$ vertices which are grouped into $n+1$ layers $L_0, L_1, \ldots, L_n$, where the layers L_0 and L_n contain 5 vertices, while each of the other layers contains 10 vertices. In Fig. 2 the case $n = 5$ is drawn, that is, C_{50}, from which the general edge structure of these graphs should be clear.

The main result of this section reads as follows.

Theorem 4.1. *If $n \geq 3$, then $C_{\mathrm{Sz}}(C_{10n}) = n+1 = O_e(C_{10n})$.*

Proof. Let $L_0, L_1, \ldots, L_n$ be the layers of vertices of C_{10n}, and let S_i be the set of edges connecting a vertex of L_{i-1} to a vertex of L_i. It is not difficult to observe that for $0 \leq i \leq \left\lfloor \frac{n+1}{2} \right\rfloor$, the edges of L_i and L_{n-i} are in the same orbit and that for $1 \leq j \leq \lfloor \frac{n}{2} \rfloor$, the edges of S_j and edges of S_{n-j} are in the same edge orbit. Hence, using Theorem 3.1, $C_{\mathrm{Sz}}(C_{10n}) \leq O_e(C_{10n}) = n+1$.

We checked by computer that $C_{\mathrm{Sz}}(C_{10n}) = n+1$ holds for $3 \leq n \leq 9$. In the rest we prove by induction that the same holds for $n \geq 9$. To simplify the notation, set $N(e) = n_u(e)n_v(e)$ for an edge $e = uv$. For $n = 9, 10$, let $e_i \in L_i$, $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$ and $f_j \in S_j$ for $1 \leq j \leq \lfloor \frac{n+1}{2} \rfloor$. With the help of computer again we have obtained the corresponding values for C_{90} and C_{100} as given in Table 1.

Let $e = uv$ be an arbitrary edge of C_{10n}. We distinguish three typical cases with respect to the position of uv.

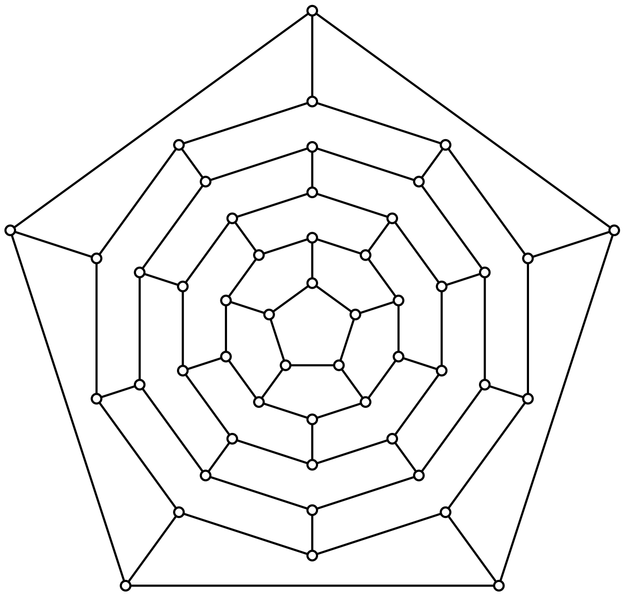

Figure 2. The C_{50} fullerene

i	$N(e_i)$	$N(f_i)$
0	12×12	-
1	18×70	9×69
2	24×64	15×75
3	32×57	25×65
4	40×49	35×55
5	-	45×45

i	$N(e_i)$	$N(f_i)$
0	12×12	-
1	18×80	9×79
2	24×74	15×85
3	32×67	25×75
4	40×59	35×65
5	50×50	45×55

Table 1. Values $N(e)$ for the edges of C_{90} (left) and of C_{100} (right)

Suppose first that uv lies within L_0 or L_{n+1}. Then for $n = 3$ one can check that $n_u(e) = 10$, while if $n \geq 4$, then $n_u(e) = 12$. The latter fact is illustrated in Fig. 3, where the vertices closer to u than to v are colored blue and the vertices closer to v than to u red.

Suppose next that $e = uv \in S_i$ for $1 \leq i \leq \lfloor \frac{n}{2} \rfloor$. Since we will consider the edge e in fullerenes C_{10n} and in $C_{10(n+1)}$, hence we specify the notation $n_u(e)$ to $n_u^{(n)}(e)$, meaning that we consider e in C_{10n}. Now we have $N_u^{(n+1)}(e) = N_u^{(n)}(e)$ and $n_v^{(n+1)}(e) = n_v^{(n)}(e) + 10$ (or vice versa). In addition, when n is odd and $uv \in S_{\lfloor \frac{n+1}{2} \rfloor}$, then $n_u^{(n)}(e) = N_v^{(n)}(e) = 5n$.

Assume finally that $uv \in L_i$, where $1 \leq i \leq \lfloor \frac{n-1}{2} \rfloor$, the vertex u is adjacent to some vertex of L_{i-1}, and the vertex v is adjacent to some vertex of L_{i+1}. Now $n_u^{(n+1)}(e) = n_v^{(n)}(e)$ and $n_v^{(n+1)}(e) = n_v^{(n)}(e) + 10$. If n is even, then for the edge $uv \in L_{\frac{n}{2}}$ we have $n_u^{(n)}(e) = N_v^{(n)}(e) = 5n$.

From the above consideration, we conclude that $C_{\mathrm{Sz}}(C_{10(n+1)}) = C_{\mathrm{Sz}}(C_{10n}) + 1 = n + 2$ which completes the inductive argument. $\square$

As a consequence of Theorem 4.1, together with a help of computer, we can also determine the Szeged index of the fullerenes C_{10n}.

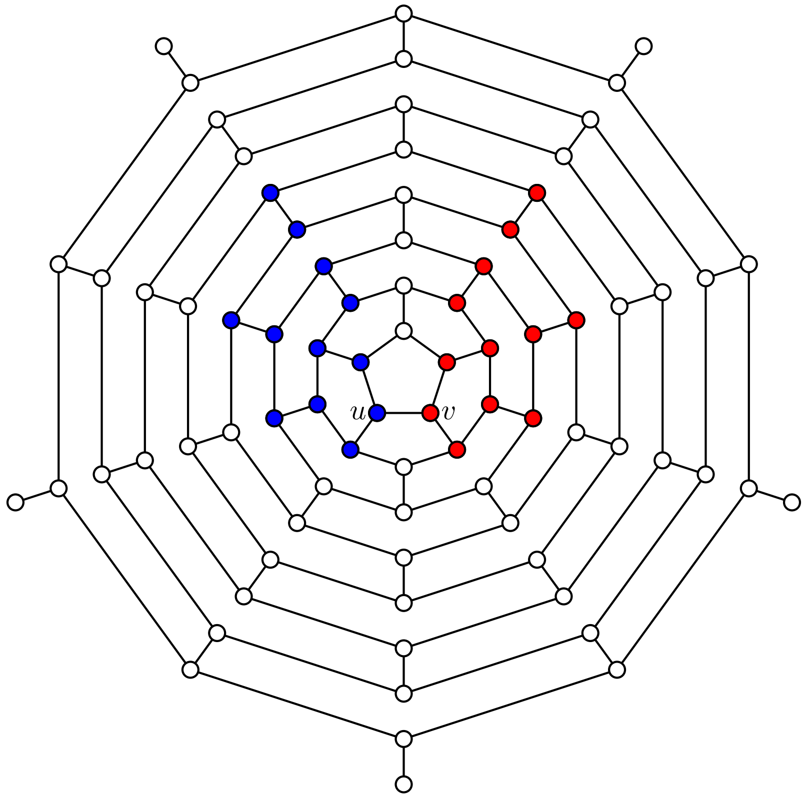

Figure 3. If $e = uv$ lies in L_0, then $n_u(e) = n_v(e) = 12$

Corollary 4.2. $\mathrm{Sz}(C_{30}) = 6655$, $\mathrm{Sz}(C_{40}) = 16830$, $\mathrm{Sz}(C_{50}) = 33545$, $\mathrm{Sz}(C_{60}) = 58900$, $\mathrm{Sz}(C_{70}) = 93535$, $\mathrm{Sz}(C_{80}) = 138810$. *Moreover, if* $n \geq 9$, *then*

$$\mathrm{Sz}(C_{10n}) = 250n^3 + 3075n - 13800.$$

5. Szeged index versus total eccentricity

The relation between the Szeged index and the Wiener index has already been well investigated. In [24] it was first proved that $\mathrm{Sz}(G) \geq W(G)$ holds for any connected graph. Moreover, the equality holds if and only if G is a block graph [11, 29]. The inequality was in [22] extended by proving that $\mathrm{Sz}(G, w) \geq W(G, w)$ holds for any connected network. In addition, in [23, 26, 27, 33] bounds on $\mathrm{Sz}(G) - W(G)$ and graphs achieving a fixed value of the difference were investigated. In this section we compare the Szeged index with the total eccentricity (cf. [30]) and prove the following result.

Theorem 5.1. *If* G *is a connected graph of order at least* 4, *then* $\mathrm{Sz}(G) \geq \mathrm{Ecc}(G)$. *Moreover, equality holds if and only if* $G = P_4$.

Proof. It is straightforward to verify that $\mathrm{Sz}(G) > \mathrm{Ecc}(G)$ holds if $G = C_n$, $n \geq 4$ or if $G = P_n$, $n \geq 5$. Moreover, $\mathrm{Sz}(P_4) = \mathrm{Ecc}(P_4) = 10$. Hence assume in the rest that G is a connected graph of order at least 4 that is neither a path nor a cycle. In particular, G contains a vertex of degree at least 3.

Let $v \in V(G)$ and let v' be a vertex with $d(v, v') = \mathrm{ecc}(v)$. Considering a shortest v, v'-path $P_{vv'}$ we infer that $d(v) \geq 1 + \cdots + \mathrm{ecc}(v)$. Moreover, since G is not a path, it contains at least one vertex that does not lie on $P_{vv'}$ and consequently

$$d(v) \geq (1 + \cdots + \mathrm{ecc}(v)) + 1 = \frac{\mathrm{ecc}(v)(\mathrm{ecc}(v)+1)}{2} + 1 \geq 2\mathrm{ecc}(v)\,,$$

where the latter inequality reduces to $\mathrm{ecc}(v)^2 + 2 \geq 3\mathrm{ecc}(v)$ which can be easily be verified to hold true.

We have thus shown that $d(v) \geq 2\mathrm{ecc}(v)$ holds for any vertex v of G. Moreover, since G contains at least one vertex, say w, of degree at least 3, by the above argument, but adding 2 instead of 1, we have $d(w) > 2\mathrm{ecc}(w)$. Therefore

$$\sum_{v \in V(G)} d(v) > \sum_{v \in V(G)} 2\mathrm{ecc}(v) = 2\mathrm{Ecc}(G)\,.$$

This implies that $W(G) > \mathrm{Ecc}(G)$. Since, as mentioned before the theorem, $\mathrm{Sz}(G) \geq W(G)$ holds for any connected graph G, we conclude that $\mathrm{Sz}(G) > \mathrm{Ecc}(G)$. □

Theorem 5.1, together by considering the graphs K_2, K_3, and P_3, yields:

Corollary 5.2. *If G is a connected graph with at least one edge, then* $\mathrm{Sz}(G) = \mathrm{Ecc}(G)$ *if and only if* $G \in \{K_3, P_4\}$.

To conclude the paper we add that a comparison between the Szeged index and the eccentric connectivity index was done in [10].

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