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Status connectivity indices and co-indices of graphs and its computation to some distance-balanced graphs

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Abstract

The status of a vertex u, denoted by $\sigma_G(u)$, is the sum of the distances between u and all other vertices in a graph G. The first and second status connectivity indices of a graph G are defined as $S_1(G) = \sum_{uv\in E(G)}[\sigma_G(u) + \sigma_G(v)]$ and $S_2(G) = \sum_{uv\in E(G)}\sigma_G(u)\sigma_G(v)$ respectively, where $E(G)$ denotes the edge set of G. In this paper we have defined the first and second status co-indices of a graph G as $\overline{S_1}(G) = \sum_{uv\notin E(G)}[\sigma_G(u) + \sigma_G(v)]$ and $\overline{S_2}(G) = \sum_{uv\notin E(G)}\sigma_G(u)\sigma_G(v)$ respectively. Relations between status connectivity indices and status co-indices are established. Also these indices are computed for intersection graph, hypercube, Kneser graph and achiral polyhex nanotorus.

Keywords: Distance in graph; Status indices; Distance-balanced graphs

1. Introduction

The graph theoretic models can be used to study the properties of molecules in theoretical chemistry. The oldest well known graph parameter is the Wiener index which was used to study the chemical properties of paraffins [1]. The Zagreb indices were used to study the structural property models [2,3]. Ramane and Yalnaik [4] obtained the status connectivity indices and analyzed its correlation with the boiling point of benzenoid hydrocarbons. In this paper we define the status co-indices of a graph and establish the relations between the status connectivity indices and status co-indices. Also we obtain the bounds for the status connectivity indices of connected complement graphs. Further we compute these status indices for intersection graph, hypercube, Kneser graph and achiral polyhex nanotorus.

Let G be a connected graph with n vertices and m edges. Let $V(G)$ be the vertex set of G and $E(G)$ be an edge set of G. The edge joining the vertices u and v is denoted by uv. The *degree* of a vertex u in a graph G is the number of

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edges incident to u and is denoted by $d_G(u)$. The *distance* between the vertices u and v is the length of shortest path joining u and v and is denoted by $d_G(u, v)$. The *diameter* of G is the maximum distance between all pair of vertices of G and is denoted by $diam(G)$.

The *status* (or *transmission*) of a vertex $u \in V(G)$, denoted by $\sigma_G(u)$ is defined as [5],

$$\sigma_G(u) = \sum_{v \in V(G)} d_G(u, v).$$

A connected graph G is *self-median* if the value $\sigma_G(u)$ is constant for all vertices u of G [6]. A graph G is *distance-balanced* if for all edges uv of G, the following equality holds [7,8],

$$|\{w \in V(G) \mid d_G(w, u) < d_G(w, v)\}| = |\{w \in V(G) \mid d_G(w, v) < d_G(w, u)\}|.$$

Balakrishnan et al. [9] noticed that the concepts of distance-balanced and self-median are the same. A connected graph is distance-balanced if and only if it is self-median.

A connected graph G is said to be *k-distance-balanced* if $\sigma_G(u) = k$ for every vertex $u \in V(G)$.

The *Wiener index* $W(G)$ of a connected graph G is defined as [1],

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v) = \frac{1}{2} \sum_{u \in V(G)} \sigma_G(u).$$

More results about Wiener index can be found in [10–16].

The first and second *Zagreb indices* of a graph G are defined as [2]

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)] \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

Results on the Zagreb indices can be found in [17–23].

The first and second *Zagreb co-indices* of a graph G are defined as [24]

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} [d_G(u) + d_G(v)] \quad \text{and} \quad \overline{M_2}(G) = \sum_{uv \notin E(G)} d_G(u) d_G(v).$$

More results on Zagreb co-indices can be found in [25,26].

The *first status connectivity index* $S_1(G)$ and *second status connectivity index* $S_2(G)$ of a graph G are defined as [4]

$$S_1(G) = \sum_{uv \in E(G)} [\sigma_G(u) + \sigma_G(v)] \quad \text{and} \quad S_2(G) = \sum_{uv \in E(G)} \sigma_G(u) \sigma_G(v). \tag{1}$$

We observe that the first status connectivity index is nothing but the degree distance of a graph introduced by Dobrynin and Kotchetova [27] and Gutman [28]. The *degree distance* of G is

$$D'(G) = \sum_{u \in V(G)} d_G(u) \sigma_G(u) = \sum_{\{u,v\} \subseteq V(G)} [d_G(u) + d_G(v)] d_G(u, v).$$

The degree distance of graphs is well studied in the literature [29–36].

Analog to Eq. (1) and the definition of Zagreb co-indices, we define the *first status co-index* $\overline{S_1}(G)$ and the *second status co-index* $\overline{S_2}(G)$ as

$$\overline{S_1}(G) = \sum_{uv \notin E(G)} [\sigma_G(u) + \sigma_G(v)] \quad \text{and} \quad \overline{S_2}(G) = \sum_{uv \notin E(G)} [\sigma_G(u) \sigma_G(v)].$$

For a graph given in Fig. 1, $S_1 = 74$, $S_2 = 169$, $\overline{S_1} = 22$ and $\overline{S_2} = 60$.

2. Status connectivity indices and co-indices

In [4] the results on status connectivity indices are obtained. In this section we obtain further results on the status connectivity indices and co-indices of graphs.

Proposition 2.1. *Let G be a connected graph on n vertices. Then*

$$\overline{S_1}(G) = 2(n-1)W(G) - S_1(G)$$

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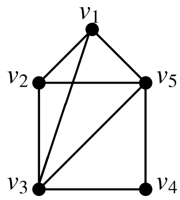

Fig. 1.

and

$$\overline{S_2}(G) = 2(W(G))^2 - \frac{1}{2}\sum_{u\in V(G)} (\sigma_G(u))^2 - S_2(G).$$

Proof.

$$\begin{aligned}\overline{S_1}(G) &= \sum_{uv\notin E(G)} [\sigma_G(u) + \sigma_G(v)]\\ &= \sum_{\{u,v\}\subseteq V(G)} [\sigma_G(u) + \sigma_G(v)] - \sum_{uv\in E(G)} [\sigma_G(u) + \sigma_G(v)]\\ &= (n-1)\sum_{u\in V(G)} \sigma_G(u) - S_1(G)\\ &= 2(n-1)W(G) - S_1(G).\end{aligned}$$

Also

$$\begin{aligned}\overline{S_2}(G) &= \sum_{uv\notin E(G)} [\sigma_G(u)\sigma_G(v)]\\ &= \sum_{\{u,v\}\subseteq V(G)} [\sigma_G(u)\sigma_G(v)] - \sum_{uv\in E(G)} [\sigma_G(u)\sigma_G(v)]\\ &= \frac{1}{2}\left[\left[\sum_{u\in V(G)} \sigma_G(u)\right]^2 - \sum_{u\in V(G)} \sigma_G(u)^2\right] - S_2(G)\\ &= 2(W(G))^2 - \frac{1}{2}\sum_{u\in V(G)} (\sigma_G(u))^2 - S_2(G).\end{aligned}$$

Corollary 2.2. *Let G be a connected graph with n vertices, m edges and $diam(G) \leq 2$. Then*

$$\overline{S_1}(G) = 2n(n-1)^2 - 6m(n-1) + M_1(G)$$

and

$$\overline{S_2}(G) = (n-1)^2\,[2n(n-1) - 8m] + 2m^2 + \left(2n - \frac{5}{2}\right) M_1(G) - M_2(G).$$

Proof. For any graph G of $diam(G) \leq 2$, $\sigma_G(u) = 2n - 2 - d_G(u)$ and

$$W(G) = m + 2\left[\frac{n(n-1)}{2} - m\right] = n(n-1) - m.$$

Also $S_1(G) = 4m(n-1) - M_1(G)$ and $S_2(G) = 4m(n-1)^2 - 2(n-1)M_1(G) + M_2(G)$ [4]. Therefore by Proposition 2.1,

$$\begin{aligned}\overline{S_1}(G) &= 2(n-1)[n(n-1) - m] - \{4m(n-1) - M_1(G)\}\\ &= 2n(n-1)^2 - 6m(n-1) + M_1(G)\end{aligned}$$

and

$$\begin{aligned}\overline{S_2}(G) &= 2[n(n-1)-m]^2 - \frac{1}{2}\sum_{u\in V(G)}(2n-2-d_G(u))^2 - \left[4m(n-1)^2 - 2(n-1)M_1(G) + M_2(G)\right]\\ &= 2[n(n-1)-m]^2 - \frac{1}{2}\left[\sum_{u\in V(G)}(2n-2)^2 - 2(2n-2)\sum_{u\in V(G)} d_G(u) + \sum_{u\in V(G)}(d_G(u))^2\right]\\ &\quad -\left[4m(n-1)^2 - 2(n-1)M_1(G) + M_2(G)\right]\\ &= 2[n(n-1)-m]^2 - \frac{1}{2}\left[n(2n-2)^2 - 4m(2n-2) + M_1(G)\right]\\ &\quad - \left[4m(n-1)^2 - 2(n-1)M_1(G) + M_2(G)\right]\\ &= (n-1)^2\,[2n(n-1)-8m] + 2m^2 + \left(2n-\frac{5}{2}\right)M_1(G) - M_2(G).\end{aligned}$$

Proposition 2.3. *Let G be a connected graph with n vertices, m edges and $diam(G) \le 2$. Then*

$$\overline{S_1}(G) = 2(n-1)\,[n(n-1)-2m] - \overline{M_1}(G)$$

and

$$\overline{S_2}(G) = 2(n-1)^2\,[n(n-1)-2m] - 2(n-1)\overline{M_1}(G) + \overline{M_2}(G).$$

Proof. For any graph G of $diam(G) \le 2$, $\sigma_G(u) = 2n-2-d_G(u)$. Therefore

$$\begin{aligned}\overline{S_1}(G) &= \sum_{uv\notin E(G)}[(2n-2-d_G(u)) + (2n-2-d_G(v))]\\ &= \left[\frac{n(n-1)}{2} - m\right](4n-4) - \sum_{uv\notin E(G)}[d_G(u)+d_G(v)]\\ &= 2(n-1)\,[n(n-1)-2m] - \overline{M_1}(G)\end{aligned}$$

and

$$\begin{aligned}\overline{S_2}(G) &= \sum_{uv\notin E(G)}[(2n-2-d_G(u))(2n-2-d_G(v))]\\ &= \left[\frac{n(n-1)}{2} - m\right](2n-2)^2 - (2n-2)\sum_{uv\notin E(G)}[d_G(u)+d_G(v)] + \sum_{uv\notin E(G)}(d_G(u)d_G(v))\\ &= 2(n-1)^2\,[n(n-1)-2m] - 2(n-1)\overline{M_1}(G) + \overline{M_2}(G).\end{aligned}$$

Proposition 2.4. *Let G be a graph with n vertices and m edges. Let $\overline{G}$ be the complement of G and it is connected. Then*

$$S_1(\overline{G}) \ge (n-1)[n(n-1)-2m] + \overline{M_1}(G)$$

and

$$S_2(\overline{G}) \ge (n-1)^2\left[\frac{n(n-1)}{2} - m\right] + (n-1)\overline{M_1}(G) + \overline{M_2}(G).$$

Equality in both cases holds if and only if $diam(\overline{G}) \le 2$.

Proof. For any vertex u in $\overline{G}$ there are $n-1-d_G(u)$ vertices which are at distance 1 and the remaining $d_G(u)$ vertices are at distance at least 2. Therefore

$$\begin{aligned}\sigma_{\overline{G}}(u) &\ge [n-1+d_G(u)] + 2d_G(u)\\ &= n-1+d_G(u).\end{aligned}$$

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Therefore,

$$\begin{aligned}
S_1(\overline{G}) &= \sum_{uv \in E(\overline{G})} \left[\sigma_{\overline{G}}(u) + \sigma_{\overline{G}}(v)\right] \\
&\geq \sum_{uv \in E(\overline{G})} [n-1+d_G(u)+n-1+d_G(v)] \\
&= \sum_{uv \notin E(G)} [2n-2+d_G(u)+d_G(v)] \\
&= \left[\frac{n(n-1)}{2} - m\right](2n-2) + \sum_{uv \notin E(G)} [d_G(u)+d_G(v)] \\
&= [n(n-1)-2m](n-1) + \overline{M_1}(G).
\end{aligned}$$

And

$$\begin{aligned}
S_2(\overline{G}) &= \sum_{uv \in E(\overline{G})} \sigma_{\overline{G}}(u)\sigma_{\overline{G}}(v) \\
&\geq \sum_{uv \in E(\overline{G})} [n-1+d_G(u)][n-1+d_G(v)] \\
&= \sum_{uv \notin E(G)} \left[(n-1)^2 + (n-1)[d_G(u)+d_G(v)] + [d_G(u)d_G(v)]\right] \\
&= \left[\frac{n(n-1)}{2} - m\right](n-1)^2 + (n-1)\overline{M_1}(G) + \overline{M_2}(G).
\end{aligned}$$

For equality: If the diameter of $\overline{G}$ is 1 or 2 then the equality holds.

Conversely, let $S_1(\overline{G}) = (n-1)[n(n-1)-2m] + \overline{M_1}(G)$.

Suppose, $diam(\overline{G}) \geq 3$, then there exists at least one pair of vertices, say u_1 and u_2 such that $d_{\overline{G}}(u_1, u_2) \geq 3$.

Therefore $\sigma_{\overline{G}}(u_1) \geq d_{\overline{G}}(u_1) + 3 + 2(n-2-d_{\overline{G}}(u_1)) = n + d_G(u_1)$. Similarly $\sigma_{\overline{G}}(u_2) \geq n + d_G(u_2)$ and for all other vertices u of $\overline{G}$, $\sigma_{\overline{G}}(u) \geq n-1+d_G(u)$.

Partition the edge set of $\overline{G}$ into three sets E_1, E_2 and E_3, where

$$E_1 = \{u_1 v \mid \sigma_{\overline{G}}(u_1) \geq n + d_G(u_1) \text{ and } \sigma_{\overline{G}}(v) \geq n-1+d_G(v)\},$$

$$E_2 = \{u_2 v \mid \sigma_{\overline{G}}(u_2) \geq n + d_G(u_2) \text{ and } \sigma_{\overline{G}}(v) \geq n-1+d_G(v)\}$$

and

$$E_3 = \{uv \mid \sigma_{\overline{G}}(u) \geq n-1+d_G(u) \text{ and } \sigma_{\overline{G}}(v) \geq n-1+d_G(v)\}.$$

It is easy to check that $|E_1| = d_{\overline{G}}(u_1)$, $|E_2| = d_{\overline{G}}(u_2)$ and $|E_3| = \binom{n}{2} - m - d_{\overline{G}}(u_1) - d_{\overline{G}}(u_2)$.

Therefore

$$\begin{aligned}
S_1(\overline{G}) &= \sum_{uv \in E(\overline{G})} \left[\sigma_{\overline{G}}(u) + \sigma_{\overline{G}}(v)\right] \\
&= \sum_{uv \in E_1} \left[\sigma_{\overline{G}}(u) + \sigma_{\overline{G}}(v)\right] + \sum_{uv \in E_2} \left[\sigma_{\overline{G}}(u) + \sigma_{\overline{G}}(v)\right] + \sum_{uv \in E_3} \left[\sigma_{\overline{G}}(u) + \sigma_{\overline{G}}(v)\right] \\
&\geq \sum_{uv \in E_1} [2n-1+d_G(u)+d_G(v)] + \sum_{uv \in E_2} [2n-1+d_G(u)+d_G(v)] \\
&\quad + \sum_{uv \in E_3} [2n-2+d_G(u)+d_G(v)] \\
&= (2n-1)d_{\overline{G}}(u_1) + (2n-1)d_{\overline{G}}(u_2) + (2n-2)\left[\binom{n}{2} - m - d_{\overline{G}}(u_1) - d_{\overline{G}}(u_2)\right]
\end{aligned}$$

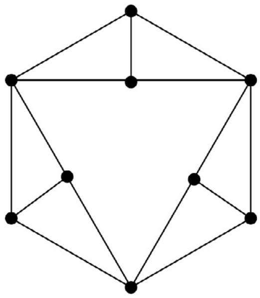

Fig. 2. The distance-balanced but not degree regular graph.

$$+ \sum_{uv \in E(\overline{G})} [d_G(u) + d_G(v)]$$

$$= (n-1)[n(n-1) - 2m] + d_{\overline{G}}(u_1) + d_{\overline{G}}(u_2) + \overline{M_1}(G),$$

which is a contradiction. Hence $diam(\overline{G}) \leq 2$.

The equality of $S_2(\overline{G})$ can be proved analogously.

3. Status connectivity indices and co-indices of some distance-balanced graphs

A bijection α on $V(G)$ is called an *automorphism* of G if it preserves $E(G)$. In other words, α is an automorphism if for each $u, v \in V(G)$, $e = uv \in E(G)$ if and only if $\alpha(e) = \alpha(u)\alpha(v) \in E(G)$. Let

$$Aut(G) = \{\alpha \mid \alpha : V(G) \longrightarrow V(G) \text{ such that } \alpha \text{ and } \alpha^{-1} \text{ preserve adjacency}\}.$$

It is known that $Aut(G)$ forms a group under the composition of mappings. A graph G is called *vertex-transitive* if for every two vertices u and v of G, there exists an automorphism α of G such that $\alpha(u) = v$. It is known that any vertex-transitive graph is vertex degree regular, distance-balanced and self-centered. The graph depicted in Fig. 2 is 14-distance-balanced graph but not degree regular and therefore not vertex-transitive (see [37,38]).

The following lemma is straightforward from the definition of status connectivity indices.

Lemma 3.1. *Let G be a connected k-distance-balanced graph with m edges. Then $S_1(G) = 2mk$ and $S_2(G) = mk^2$.*

Theorem 3.2 (*[39]*)**.** *Let G be a connected graph on n vertices with the automorphism group $Aut(G)$ and the vertex set $V(G)$. Let $V_1, V_2, \ldots, V_t$ be all orbits of the action $Aut(G)$ on $V(G)$. Suppose that for each $1 \leq i \leq t$, k_i are the status of vertices in the orbit V_i. Then*

$$W(G) = \frac{1}{2} \sum_{i=1}^{t} |V_i| k_i.$$

Specially, if G is vertex-transitive (that is, $t = 1$), then $W(G) = \frac{1}{2} nk$, where k is the status of each vertex of G.

Analogous to Theorem 3.2 and as a consequence of Proposition 2.1, we have the following.

Theorem 3.3. *Let G be a connected graph on n vertices with the automorphism group $Aut(G)$ and the vertex set $V(G)$. Let $V_1, V_2, \ldots, V_t$ be all orbits of the action $Aut(G)$ on $V(G)$. Suppose that for each $1 \leq i \leq t$, d_i and k_i are the vertex degree and the status of vertices in the orbit V_i, respectively. Then*

$$S_1(G) = \sum_{i=1}^{t} |V_i| d_i k_i \quad \text{and} \quad \overline{S_1}(G) = (n-1) \sum_{i=1}^{t} \left[|V_i| k_i \left(1 - \frac{d_i}{n-1}\right)\right].$$

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Specially, if G is vertex-transitive (that is, $t = 1$), then

$$S_1(G) = ndk, \quad S_2(G) = \frac{1}{2}ndk^2,$$

$$\overline{S_1}(G) = 2\binom{n}{2}k - ndk, \quad \overline{S_2}(G) = \left[\binom{n}{2} - \frac{nd}{2}\right]k^2,$$

where d and k are the degree and the status of each vertex of G respectively.

The following is a direct consequence of Proposition 2.1, Lemma 3.1 and Theorem 3.2.

Lemma 3.4. *Let G be a connected k-distance-balanced graph with m edges. Then*

$$\overline{S_1}(G) = 2\binom{n}{2}k - 2mk \quad \text{and} \quad \overline{S_2}(G) = \binom{n}{2}k^2 - mk^2.$$

Let S be a set and $F = \{S_1, \ldots, S_q\}$ be a non-empty family of distinct non-empty subsets of S such that $S = \bigcup_{i=1}^{q} S_i$. The *intersection graph* [40] of S which is denoted by $\Omega(F)$ has F as its set of vertices and two distinct vertices S_i and S_j, $i \neq j$, are adjacent if and only if $S_i \bigcap S_j \neq \emptyset$. Here we will consider a set S of cardinality p and let F be the set of all subsets of S of cardinality t, $1 < t < p$, which is denoted by $S^{\{t\}}$. Upon convenience we may set $S = \{1, 2, \ldots, p\}$. Let us denote the intersection graph $\Omega(S^{\{t\}})$ by $\Gamma^{\{t\}} = (V, E)$. The number of vertices of this graph is $|V| = \binom{p}{t}$ and the degree d of each vertex is as follows:

$$d = \begin{cases} \binom{p}{t} - \binom{p-t}{t} - 1, & p \geq 2t; \\ \binom{p}{t} - 1, & p < 2t. \end{cases}$$

The number of its edges is as follows:

$$|E| = \begin{cases} \frac{1}{2}\binom{p}{t}\left[\binom{p}{t} - \binom{p-t}{t} - 1\right], & p \geq 2t; \\ \frac{1}{2}\binom{p}{t}\left[\binom{p}{t} - 1\right], & p < 2t. \end{cases}$$

Lemma 3.5 (*[41]*)**.** *The intersection graph $\Gamma^{\{t\}}$ is vertex-transitive and for any t-element subset A of S we have*

$$\sigma_{\Gamma^{\{t\}}}(A) = \begin{cases} \binom{p}{t} + \binom{p-t}{t} - 1, & p \geq 2t; \\ \binom{p}{t} - 1, & p < 2t. \end{cases}$$

Moreover,

$$W(\Gamma^{\{t\}}) = \begin{cases} \frac{1}{2}\binom{p}{t}\left(\binom{p}{t} + \binom{p-t}{t} - 1\right), & p \geq 2t; \\ \frac{1}{2}\binom{p}{t}\left(\binom{p}{t} - 1\right), & p < 2t. \end{cases}$$

Theorem 3.6. *For intersection graph $\Gamma^{\{t\}}$,*

$$S_1(\Gamma^{\{t\}}) = \begin{cases} \binom{p}{t}\left(\binom{p}{t} - \binom{p-t}{t} - 1\right)\left(\binom{p}{t} + \binom{p-t}{t} - 1\right), & p \geq 2t; \\ \binom{p}{t}\left(\binom{p}{t} - 1\right)^2, & p < 2t. \end{cases}$$

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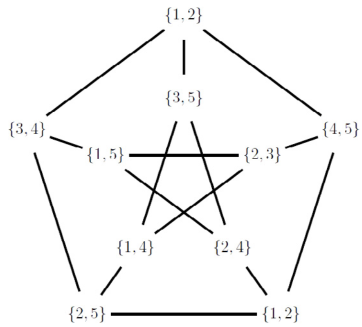

Fig. 3. The odd graph $O_3 = KG_{5,2}$.

$$S_2(\Gamma^{\{t\}}) = \begin{cases} \frac{1}{2}\binom{p}{t}\left(\binom{p}{t} - \binom{p-t}{t} - 1\right)\left(\binom{p}{t} + \binom{p-t}{t} - 1\right)^2, & p \geq 2t; \\ \frac{1}{2}\binom{p}{t}\left(\binom{p}{t} - 1\right)^3, & p < 2t. \end{cases}$$

$$\overline{S_1}(\Gamma^{\{t\}}) = \begin{cases} \binom{p-t}{t}\binom{p}{t}\left(\binom{p}{t} + \binom{p-t}{t} - 1\right), & p \geq 2t; \\ 2\binom{\binom{p}{t}}{2}\left(\binom{p}{t} - 1\right) - \binom{p}{t}\left(\binom{p}{t} - 1\right)^2, & p < 2t. \end{cases}$$

$$\overline{S_2}(\Gamma^{\{t\}}) = \begin{cases} \left[\binom{\binom{p}{t}}{2} - \frac{1}{2}\binom{p}{t}\left(\binom{p}{t} - \binom{p-t}{t} - 1\right)\right]\left(\binom{p}{t} + \binom{p-t}{t} - 1\right)^2, & p \geq 2t; \\ \left[\binom{\binom{p}{t}}{2} - \frac{1}{2}\binom{p}{t}\left(\binom{p}{t} - 1\right)\right]\left(\binom{p}{t} - 1\right)^2, & p < 2t. \end{cases}$$

Proof. It is a direct consequence of Theorem 3.3 and Lemma 3.5.

The vertex set of the *hypercube* H_n consists of all n-tuples $(b_1, b_2, \ldots, b_n)$ with $b_i \in \{0, 1\}$. Two vertices are adjacent if the corresponding tuples differ in precisely one place. Moreover, H_n has exactly $2n$ vertices and $n2^{n-1}$ edges. Darafsheh [41] proved that H_n is vertex-transitive and for every vertex u, $\sigma_{H_n}(u) = n2^{n-1}$. Therefore, by Lemmas 3.1 and 3.4 we have following result.

Theorem 3.7. *For hypercube* H_n,

$$S_1(G) = n^2 2^{2n-1} \quad \text{and} \quad S_2(G) = n^3 2^{3n-3},$$

$$\overline{S_1}(G) = n^2 2^n (2n - 1 - 2^{n-1}) \quad \text{and} \quad \overline{S_2}(G) = n^3 2^{2n-2}(2n - 1 - 2^{n-1}).$$

The *Kneser graph* $KG_{p,k}$ is the graph whose vertices correspond to the k-element subsets of a set of p elements, and where two vertices are adjacent if and only if the two corresponding sets are disjoint. Clearly we must impose the restriction $p \geq 2k$. The Kneser graph $KG_{p,k}$ has $\binom{p}{k}$ vertices and it is regular of degree $\binom{p-k}{k}$. Therefore the number of edges of $KG_{p,k}$ is $\frac{1}{2}\binom{p}{k}\binom{p-k}{k}$ (see [42]). The Kneser graph $KG_{n,1}$ is the *complete graph* on n vertices. The Kneser graph $KG_{2p-1,p-1}$ is known as the *odd graph* O_p. The odd graph $O_3 = KG_{5,2}$ is isomorphic to the *Petersen graph* (see Fig. 3).

Lemma 3.8 (*[42]*). *The Kneser graph* $KG_{p,k}$ *is vertex-transitive and for each k-subset A*, $\sigma_{KG_{p,k}}(A) = \frac{2W(KG_{p,k})}{\binom{p}{k}}$.

Following proposition follows from Lemmas 3.8 and 3.1.

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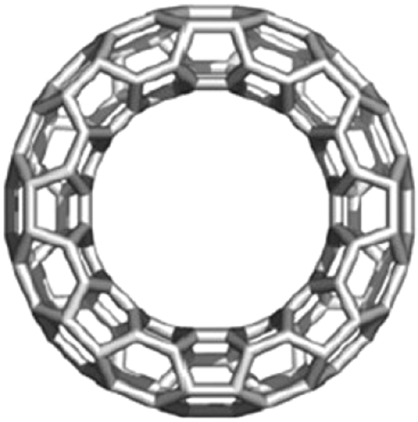

Fig. 4. A achiral polyhex nanotorus (or toroidal fullerenes) $T[p, q]$.

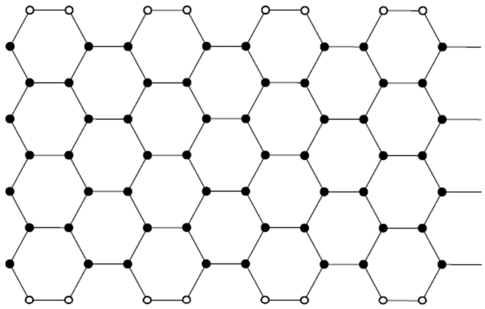

Fig. 5. A 2-dimensional lattice for an achiral polyhex nanotorus $T[p, q]$.

Proposition 3.9. *For a Kneser graph $KG_{p,k}$ we have*

$$S_1(KG_{p,k}) = 2W(KG_{p,k})\binom{p-k}{k}$$

and

$$S_2(KG_{p,k}) = \binom{p-k}{k}\left[\frac{2(W(KG_{p,k}))^2}{\binom{p}{k}}\right].$$

Following proposition follows from Proposition 2.1, Lemma 3.8 and Proposition 3.9.

Proposition 3.10. *For a Kneser graph $KG_{p,k}$ we have*

$$\overline{S_1}(KG_{p,k}) = 2W(KG_{p,k})\left[\binom{p}{k} - \binom{p-k}{k} - 1\right]$$

and

$$\overline{S_2}(KG_{p,k}) = 2(W(KG_{p,k}))^2 - W(KG_{p,k}) - \binom{p-k}{k}\left[\frac{2(W(KG_{p,k}))^2}{\binom{p}{k}}\right].$$

A nanostructure called *achiral polyhex nanotorus* (or *toroidal fullerenes*) of perimeter p and length q, denoted by $T[p, q]$ is depicted in Fig. 4 and its 2-dimensional molecular graph is in Fig. 5. It is regular of degree 3 and has pq vertices and $\frac{3pq}{2}$ edges.

The following lemma was proved in [39,43].

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Lemma 3.11 ([39,43]). *The achiral polyhex nanotorus $T = T[p,q]$ is vertex-transitive such that for an arbitrary vertex $u \in V(T)$,*

$$\sigma_T(u) = \begin{cases} \frac{q}{12}(6p^2+q^2-4), & q < p; \\ \frac{p}{12}(3q^2+3pq+p^2-4), & q \geq p. \end{cases}$$

The following is a direct consequence of Lemmas 3.1 and 3.11.

Corollary 3.12. *Let $T = T[p,q]$ be a achiral polyhex nanotorus. Then*

$$S_1(T) = \begin{cases} \frac{pq^2}{4}(6p^2+q^2-4), & q < p; \\ \frac{p^2q}{4}(3q^2+3pq+p^2-4), & q \geq p \end{cases}$$

and

$$S_2(T) = \begin{cases} \frac{pq^3}{96}(6p^2+q^2-4)^2, & q < p; \\ \frac{p^3q}{96}(3q^2+3pq+p^2-4)^2, & q \geq p. \end{cases}$$

Corollary 3.13. *Let $T = T[p,q]$ be a achiral polyhex nanotorus. Then*

$$\overline{S_1}(T) = \begin{cases} \frac{pq^2}{12}(pq-4)(6p^2+q^2-4), & q < p; \\ \frac{p^2q}{12}(pq-4)(3q^2+3pq+p^2-4), & q \geq p \end{cases}$$

and

$$\overline{S_2}(T) = \begin{cases} \frac{pq^3}{288}(pq-4)(6p^2+q^2-4)^2, & q < p; \\ \frac{p^3q}{288}(pq-4)(3q^2+3pq+p^2-4)^2, & q \geq p. \end{cases}$$

Proof. Since $2W(G) = \sum_{u \in V(G)} \sigma_G(u)$ and polyhex nanotorus $T[p,q]$ has pq vertices, by Lemma 3.11, the Wiener index of polyhex nanotorus $T[p,q]$ is as follows [43]:

$$W(T) = \begin{cases} \frac{pq^2}{24}(6p^2+q^2-4), & q < p; \\ \frac{p^2q}{24}(3q^2+3pq+p^2-4), & q \geq p. \end{cases}$$

Substituting this and Corollary 3.12 in Proposition 2.1 we get the results.

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