On the transmission-based graph topological indices

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Abstract

The distance $d(u, v)$ between the vertices $u$ and $v$ of a connected graph $G$ is defined as the number of edges in a minimal path connecting them. The \textit{transmission} of a vertex $v$ of $G$ is defined by $\sigma(v) = \sum_{u \in V(G)} d(v, u)$. In this article we aim to define some transmission-based topological indices. We obtain lower and upper bounds on these indices and characterize graphs for which these bounds are best possible. Finally, we find these indices for various graphs using the group of automorphisms of $G$. This is an efficient method of finding these indices especially when the automorphism group of $G$ has a few orbits on $V(G)$ or $E(G)$.

\textbf{Key words:} Graph distance, Topological index, Transmission

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1 Introduction and Preliminaries

Let $G$ be a simple connected graph with the finite vertex set $V(G)$ and the edge set $E(G)$, and denote by $n = |V(G)|$ and $m = |E(G)|$ the number of vertices and edges, respectively.
Using the standard terminology in graph theory, we refer the reader to [42]. The degree \( d(u) \) of the vertex \( u \in V(G) \) is the number of the edges incident to \( u \). The edge of the graph \( G \) connecting the vertices \( u \) and \( v \) is denoted by \( uv \).

The role of molecular descriptors (especially topological descriptors) is remarkable in mathematical chemistry especially in QSPR/QSAR investigations. In mathematical chemistry, the first Zagreb index \( M_1(G) \) and the second Zagreb index \( M_2(G) \) belong to the family of the most important degree-based molecular descriptors. They are defined as [22], [23], [25], [31], [36]

\[
M_1(G) = \sum_{uv \in E(G)} d(u) + d(v) = \sum_{u \in V(G)} d^2(u), \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).
\]

Similarly, the first variable Zagreb index and the second variable Zagreb index are defined as [33], [36], [44]

\[
M_1^\lambda(G) = \sum_{u \in V(G)} d(u)^{2\lambda}, \quad M_2^\lambda(G) = \sum_{uv \in E(G)} d(u)^\lambda d(v)^\lambda,
\]

where \( \lambda \) is a real number.

The Randic index \( R(G) \), the ordinary sum-connectivity index \( X(G) \), the harmonic index \( H(G) \) and geometric-arithmetic index \( GA(G) \) are also widely used degree-based topological indices [39], [48], [17], [43], [46], [47]. By definition,

\[
R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}, \quad X(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) + d(v)}},
\]

\[
H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}, \quad GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}.
\]

Let \( \Delta = \Delta(G) \) and \( \delta = \delta(G) \) be the maximum and the minimum degrees, respectively, of vertices of \( G \). The average degree of \( G \) is \( \frac{2m}{n} \). A connected graph \( G \) is said to be bidegreed
with degrees $\Delta$ and $\delta$ ($\Delta > \delta \geq 1$), if at least one vertex of $G$ has degree $\Delta$ and at least one vertex has degree $\delta$, and if no vertex of $G$ has degree different from $\Delta$ or $\delta$. A connected bidegreed bipartite graph is called semi-regular if each vertex in the same part of a bipartition has the same degree. A graph $G$ is called regular if all its vertices have the same degree, otherwise it is said to be irregular. In many applications and problems in theoretical chemistry, it is important to know how a given graph is irregular. The (vertex) regularity of a graph is defined in several approaches. Two most frequently used graph topological indices that measure how irregular a graph is, are the irregularity and variance of degrees. Let $\text{imb}(e) = |d(u) - d(v)|$ be the imbalance of an edge $e = uv \in E(G)$. In [1], the irregularity of $G$, which is a measure of irregularity of graph $G$, defined as

$$\text{irr}(G) = \sum_{e \in E(G)} \text{imb}(e) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|. \quad (1)$$

The variance of degrees of graph $G$ is defined as [7]

$$\text{Var}(G) = \frac{1}{n} \sum_{u \in V(G)} \left( d(u) - \frac{2m}{n} \right)^2 = \frac{M_1(G)}{n} - \frac{4m^2}{n^2}. \quad (2)$$

Another measure of irregularity, which is called degree deviation, defined as [37]

$$s(G) = \sum_{u \in V(G)} \left| d(u) - \frac{2m}{n} \right|. \quad (3)$$

It is worth mentioning that $\frac{s(G)}{n}$ is noting but the mean deviation of the data set $\{d(u) \mid u \in V(G)\}$.

The distance between the vertices $u$ and $v$ in graph $G$ is denoted by $d(u, v)$ and it is defined as the number of edges in a minimal path connecting them. The eccentricity $\varepsilon(v)$ of a vertex $v$ is the maximum distance from $v$ to any other vertex. The diameter $\text{diam}(G)$ of $G$ is the maximum eccentricity among the vertices of $G$. The transmission (or status) of a vertex

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$v$ of $G$ is defined as $\sigma(v) = \sigma_G(v) = \sum_{u \in V(G)} d(v, u)$. A graph $G$ is said to be transmission regular [3] if $\sigma(u) = \sigma(v)$ for any vertex $u$ and $v$ of $G$. A transmission regular graph $G$ is called $k$-transmission regular if there exists a positive integer $k$, for which $\sigma(v) = k$ for any vertex $v$ of $G$. In $K_n$, the complete graph of order $n$, each vertex has transmission $n - 1$. So it is $(n - 1)$-transmission regular. The cycle $C_n$ and the complete bipartite graph $K_{a,a}$ are transmission regular. It has been verified that there exist regular and non-regular transmission regular graphs [3]. Consider the polyhedron depicted in Figure 1. It is the rhombic dodecahedron that contains 14 vertices, (8 vertices of degree 3 and 6 vertices of degree 4), 24 edges and 12 faces, all of them are congruent rhombi.

![Figure 1: The rhombic dodecahedron](image)

The graph $G_{RD}$ of the rhombic dodecahedron is a bidegreed, semi-regular 28-transmission regular graph (See Figure 2). An interesting observation is that the 14-vertex polyhedral graph $G_{RD}$ depicted in Figure 2 is identical to the semi-regular graph published earlier in an alternative form in [3]. It is conjectured that $G_{RD}$ is the smallest non-regular, bipartite, polyhedral (3-connected) and transmission regular graph.
If \( \omega \) is a vertex weight of graph \( G \), then one can see that

\[
\sum_{\{u,v\} \subseteq V(G)} (\omega(u) + \omega(v))d(u,v) = \sum_{v \in V(G)} \omega(v)\sigma(v). \tag{3}
\]

It is easy to construct various transmission-based indices having the same structure as the known degree-based topological indices. Based on this analogy-concept, the corresponding transmission-based indices are defined.

Let us define the transmission Randić index \( RS(G) \), the transmission ordinary sum-connectivity index \( XS(G) \), the transmission harmonic index \( HS(G) \) and the transmission geometric-arithmetic index \( GAS(G) \) as follows:

\[
RS(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma(u)\sigma(v)}}, \quad XS(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma(u) + \sigma(v)}},
\]

\[
HS(G) = \sum_{uv \in E(G)} \frac{2}{\sigma(u) + \sigma(v)}, \quad GAS(G) = \frac{n}{2m} \sum_{uv \in E(G)} \frac{2\sqrt{\sigma(u)\sigma(v)}}{\sigma(u) + \sigma(v)}.
\]

It follows that \( GAS(G) \leq \frac{n}{2} \), with equality if and only if \( G \) is a transmission regular graph.

The Wiener index \( W(G) \), the Balaban index \( J(G) \) and the sum-Balaban index \( SJ(G) \) represent a particular class of transmission-based topological indices. They are defined as
\[ W(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d(u, v) = \frac{1}{2} \sum_{u \in V(G)} \sigma(u), \]

\[ J(G) = \frac{m}{m - n + 2} \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma(u)\sigma(v)}} = \frac{m}{m - n + 2} RS(G), \]

\[ SJ(G) = \frac{m}{m - n + 2} \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma(u) + \sigma(v)}} = \frac{m}{m - n + 2} XS(G). \]

In [40] the first transmission Zagreb index \( MS_1(G) \) and the second transmission Zagreb index \( MS_2(G) \) are defined as

\[ MS_1(G) = \sum_{uv \in E(G)} \sigma(u) + \sigma(v) = \sum_{u \in V(G)} d(u)\sigma(u), \quad MS_2(G) = \sum_{uv \in E(G)} \sigma(u)\sigma(v). \]

It is important to note that \( MS_1(G) \) coincides with the degree distance \( DD(G) \) that was introduced in [11], [24] and [41]. In fact by Eq. (3),

\[ DD(G) = \sum_{\{u,v\} \subseteq V(G)} (d(u) + d(v))d(u, v) = \sum_{v \in V(G)} d(v)\sigma(v) = MS_1(G). \quad (4) \]

Consequently, if \( G \) is a \( k \)-transmission regular graph with \( m \) vertices, then \( DD(G) = MS_1(G) = 2mk \).

Let us propose the variable degree transmission Zagreb index \( MSD^\lambda(G) \) and the variable transmission Zagreb index \( MS^\lambda(G) \) as follows

\[ MSD^\lambda(G) = \sum_{u \in V(G)} d(u)\sigma(u)^{2\lambda-1}, \quad MS^\lambda(G) = \sum_{u \in V(G)} \sigma(u)^{2\lambda}, \]
where $\lambda$ is a real number.

The eccentric distance sum of a graph $G$, denoted by $\xi^d(G)$, defined as [20]

$$\xi^d(G) = \sum_{u \in V(G)} \varepsilon(u)\sigma(u).$$

It follows from Eq. (3) that

$$\xi^d(G) = \sum_{\{u,v\} \subseteq V(G)} (\varepsilon(u) + \varepsilon(v))d(u,v) = \sum_{v \in V(G)} \varepsilon(v)\sigma(v).$$  \hspace{1cm} (5)

Inspired from Eq. (6) and Eq. (7) we define two transmission-based irregularity as follows:
Let $G$ be a connected graph with $n$ vertices and $m$ edges. The transmission imbalance of an edge $e = uv \in E(G)$ is defined as $\text{imb}_{Tr}(e) = |\sigma_G(u) - \sigma_G(v)|$. Let us define the transmission irregularity $\text{irr}_{Tr}(G)$ and the transmission variance $\text{Var}_{Tr}(G)$ of $G$ as follows:

$$\text{irr}_{Tr}(G) = \sum_{e \in E(G)} \text{imb}_{Tr}(e) = \sum_{uv \in E(G)} |\sigma_G(u) - \sigma_G(v)|.$$  \hspace{1cm} (6)

$$\text{Var}_{Tr}(G) = \frac{1}{n} \sum_{u \in V(G)} \left( \sigma_G(u) - \frac{2W(G)}{n} \right)^2 = \frac{MSD^1(G)}{n} - \frac{4W(G)^2}{n^2} \geq 0.$$  \hspace{1cm} (7)

Note that $\frac{2W(G)}{n}$ is nothing but the vertex transmission average of graph $G$. It is obvious that $\text{Var}_{Tr}(G)$ is equal to zero if and only if $G$ is transmission regular.

Let us also define the transmission-based topological indices $QS_e(G)$ and $QS_{v,e}(G)$ as follows

$$QS_e(G) = \frac{1}{m} \text{irr}_{Tr}(G), \quad QS_{v,e}(G) = \frac{n}{2} \left\{ 1 + \frac{1}{m} \text{irr}_{Tr}(G) \right\} = \frac{n}{2} \left\{ 1 + QS_e(G) \right\}.$$ 

**Remark 1.** Let $G$ be an $n$-vertex graph. Comparing topological indices GAS$(G)$ and $QS_{v,e}(G)$,
we get
\[ \text{GAS}(G) \leq \frac{n}{2} \leq QS_{v,e}(G). \]

Equalities hold in both sides simultaneously if and only if \( G \) is transmission regular.

## 2 Establishing lower and upper bounds

**Lemma 1.** Let \( G \) be a connected graph with \( n \geq 2 \) vertices and \( m \) edges. Then

\[ 0 \leq \text{irr}_{Tr}(G) \leq m(n-2), \]

\[ 0 \leq \sum_{uv \in E(G)} (\sigma(u) - \sigma(v))^2 \leq m(n-2)^2. \]

The equality on the right-hand sides holds if and only if \( G \) is isomorphic to \( S_n \). The equality on the left-hand sides holds if and only if \( G \) is transmission regular.

**Proof.** For an arbitrary edge \( uv \) of \( G \), we have \( |\sigma(u) - \sigma(v)| \leq n-2 \). Therefore,

\[ \text{irr}_{Tr}(G) = \sum_{uv \in E(G)} |\sigma(u) - \sigma(v)| \leq \sum_{uv \in E(G)} (n-2) = m(n-2). \]

It is trivial that in both formulas the equality on the right-hand side holds if and only if \( G \) isomorphic to \( S_n \), since the star is the only graph where equality holds for each edge. \( \square \)

**Corollary 1.** Let \( T \) be a tree with \( n \geq 2 \) vertices. Then

\[ 0 \leq \text{irr}_{Tr}(T) \leq (n-1)(n-2), \]

\[ 0 \leq \sum_{uv \in E(T)} (\sigma(u) - \sigma(v))^2 \leq (n-1)(n-2)^2. \]
The equality on the right-hand sides holds if and only if $G$ is isomorphic to $S_n$. The equality on the left-hand sides holds if and only if $G$ is transmission regular.

Proof. It is a consequence of Lemma 1 and the fact that a tree with $n$ vertices has exactly $n - 1$ edges.

**Corollary 2.** Let $G$ be a connected graph with $n \geq 2$ vertices. Then

\[
(n - 2) \geq QS_e(G) \geq 0
\]

and

\[
\frac{n(n-1)}{2} \geq QS_{v,e}(G) \geq \frac{n}{2}.
\]

The upper bounds are achieved if and only if $G$ is isomorphic to $S_n$ and the lower bounds are achieved if and only if $G$ is transmission regular.

Proof. It is a direct consequence of Lemma 1.

**Lemma 2.** Let $G$ be a connected graph with $n \geq 3$ vertices and with maximum vertex degree $\Delta$. Then for each arbitrary vertex $u$ of $G$ 

\[
\sigma(u) \geq 2(n-1) - d(u) \geq 2(n-1) - \Delta \geq n - 1.
\]

Proof. Because $n - 1 \geq \Delta \geq d(u)$ one obtains that

\[
\sigma(u) = \sum_{\{w \in V|d(u,w)=1\}} d(u,w) + \sum_{\{w \in V|d(u,w)>1\}} d(u,w) = d(u) + \sum_{\{w \in V|d(u,w)>1\}} d(u,w)
\]

\[
\geq d(u) + 2(n - 1 - d(u)) = 2n - 2 - d(u) \geq 2(n - 1) - \Delta \geq n - 1.
\]
Remark 2. There are several graphs containing a vertex $u$ for which $\sigma(u) = n - 1$. For example, $\sigma(u) = d(u) = n - 1$ for any vertex $u$ of a complete graph $K_n$.

Remark 3. Let $G$ be a connected graph. It is easy to see that for any $u \in V(G)$, $\sigma(u) \geq 2(n - 1) - d(u)$, with equality if and only if $\varepsilon(u) \leq 2$. This implies that

(i) $\sigma(u) = 2(n-1)-d(u)$ for any vertex $u$ of a connected graph $G$ if and only if $\text{diam}(G) \leq 2$.

(ii) Let $G$ be a connected graph with $\text{diam}(G) \leq 2$. Then $G$ is transmission regular if and only if $G$ is regular.

Proposition 1. Let $G$ be a connected graph with $n$ vertices. Then

$$MSD^3_2(G) \geq 2(n-1)MS^1_1(G) - MS^3_2(G),$$

with equality if and only if $\text{diam}(G) \leq 2$.

Proof. It follows from Lemma 2 that

$$\sum_{u \in V(G)} d(u)\sigma^2(u) \geq \sum_{u \in V(G)} (2n - 2 - \sigma(u))\sigma^2(u) = 2(n-1)\sum_{u \in V(G)} \sigma^2(u) - \sum_{u \in V(G)} \sigma^3(u),$$

and by Remark 2, the equality holds if and only if $\text{diam}(G) \leq 2$. \qed

Proposition 2. Let $G$ be a connected graph with $n$ vertices. Then

$$MS_1(G) \geq 4(n-1)W(G) - MS^1_1(G),$$

with equality if and only if $\text{diam}(G) \leq 2$. 

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Proof. It follows from Lemma 2 that

\[ \sum_{u \in V(G)} d(u)\sigma(u) \geq \sum_{u \in V(G)} (2n - 2 - \sigma(u))\sigma(u) = 2(n - 1) \sum_{u \in V(G)} \sigma(u) - \sum_{u \in V(G)} \sigma^2(u). \]

It follows from Remark 3 that the equality holds if and only if diam(G) \leq 2.

Lemma 3. Let G be a connected graph with n vertices and m edges. If diam(G) \leq 2, then

(i) \( \text{irr}_{\text{Tr}}(G) = \text{irr}(G) \geq 0. \)

(ii) \( \text{QS}_{v,e}(G) = \frac{n}{2} \{ 1 + \frac{1}{m} \text{irr}(G) \} \geq \frac{n}{2}. \)

In particular, in both cases equality holds if and only if G is regular.

Proof. (i) It is a direct consequence of Lemma 1 and Remark 3. (ii) It follows directly from part (i).

Corollary 3. Let \( K_{p,q} \) be the complete bipartite graph with p + q vertices and with parts of size p and q. Then

(i) \( \text{irr}_{\text{Tr}}(K_{p,q}) = pq |p - q| \geq 0. \)

(ii) \( \text{QS}_{v,e}(K_{p,q}) = \frac{p+q}{2} \{ 1 + |p - q| \} \geq \frac{p+q}{2}, \) Specially \( \text{QS}_{v,e}(S_n) = \frac{n(n-1)}{2}. \)

In particular, the equalities in (i) and (ii) hold if and only if p = q.

Proof. (i) Since diam\( (K_{p,q}) = 2 \) and \( |E(K_{p,q})| = pq, \) it follows from Lemma 3 (i) that \( \text{irr}_{\text{Tr}}(K_{p,q}) = \text{irr}(K_{p,q}) = \sum_{uv \in E(K_{p,q})} |p - q| = pq |p - q|. \) (i) Since diam\( (K_{p,q}) = 2 \) and \( |V(K_{p,q})| = p + q, \) it follows from Lemma 3 (ii) that

\[ \text{QS}_{v,e}(K_{p,q}) = \frac{p+q}{2} \{ 1 + |p - q| \} \geq \frac{p+q}{2}. \]
Specially, let \( n \geq 2 \) and \( p = 1 \) and \( q = n - 1 \). Then \( K_{p,q} \) is isomorphic to the star \( S_n \), \( (n = p + q) \). Consequently, we obtain that

\[
QS_{v,e}(S_n) = \frac{n}{2} (1 + |2 - n|) = \frac{n(n - 1)}{2}.
\]

It follows from Lemma 3 that the equalities in (i) and (ii) hold if and only if \( K_{p,q} \) is regular if and only if \( p = q \). \( \square \)

An edge \( uv \) of a connected graph \( G \) is said to be a \textit{strong edge} of \( G \), if \( |d(u) - d(v)| > 0 \). Denote by \( es(G) \) the number of strong edges of \( G \). It is obvious that if \( G \) is a connected graphs, then \( es(G) = 0 \) if and only if \( G \) is regular. From this observation it follows that the topological invariant \( es(G) \) can be considered as a graph irregularity index. There are several graphs in which each edge is strong, that is \( es(G) = |E(G)| \). For example, \( es(K_{p,q}) = |E(K_{p,q})| = pq \) if \( p \) is not equal to \( q \). It can be easily constructed a tree graph \( T \) with an arbitrary large edge number \( m(T) \), for which \( es(T) = m(T) \). Consider the \( (n \geq 5) \)-vertex windmill graph denoted by \( W_d(n) \). It is a graph with diameter 2, with the vertex number \( n = 2k + 1 \) and with the edge number \( m = 3k \), where \( k \geq 2 \) is an arbitrary positive integer. Note that \( es(W_d(n)) = 2k = \frac{2}{3}m = n - 1 \).

**Proposition 3.** For the windmill graph \( W_d(n) \) we have

(i) \( \text{irr}_{Tv}(W_d(n)) = es(W_d(n))(n - 3) = \frac{2}{3}m(n - 3) = (n - 1)(n - 3) \).

(ii) \( QS_{v,e}(W_d(n)) = \frac{n}{2} \left\{ 1 + \frac{2}{3}(n - 3) \right\} \).

**Proof.** (i) Let \( E_0 \) be the set of strong edges of \( W_d(n) \). It is easy to see that

\[
E_0 = \left\{ uv \in E(W_d(n)) \mid d(u) = 2, d(v) = n - 1 \right\}, \quad es(W_d(n)) = |E_0|.
\]
Since diam(W_d(n)) = 2, it follows from Lemma 3 (i) that

\[ \text{irr}_{\text{Tr}}(W_d(n)) = \sum_{uv \in E_0} |d(u) - d(v)| = \sum_{uv \in E_0} |2 - (n - 1)| \]

\[ = es(W_d(n)) |2 - (n - 1)| \]

\[ = \frac{2}{3} m(n - 3) = (n - 1)(n - 3). \]

(ii) It follows from part (i) that

\[ QS_{v,e}(W_d(n)) = \frac{n}{2} \left\{ 1 + \frac{1}{m} \text{irr}_{\text{Tr}}(W_d(n)) \right\} = \frac{n}{2} \left\{ 1 + \frac{2}{3} (n - 3) \right\} \]

\[ = \frac{n}{2} \left\{ 1 + \frac{1}{m} (n - 1)(n - 3) \right\}. \]

\[ \square \]

Lemma 4 ([32]). Let P_n be a path of order n, and let V(P_n) = \{v_0, v_1, \ldots, v_{n-1}\} such that E(P_n) = \{v_i v_{i+1} | i = 0, \ldots, n - 2\}. Then for 0 \leq i \leq n - 1

\[ \sigma_{P_n}(v_i) = \frac{1}{2} \left( 2i^2 - 2(n - 1)i + (n - 1)^2 + (n - 1) \right). \]

The following is a direct consequence of Lemma 4.

Proposition 4. The transmission irregularity index of P_n is given by

\[ \text{irr}_{\text{Tr}}(P_n) = \begin{cases} 
\frac{n(n-1)}{2}, & \text{if } n \text{ is even,} \\
\frac{(n-1)^2}{2}, & \text{if } n \text{ is odd.}
\end{cases} \]

For an edge uv of a connected graph G, define the positive integers N_u and N_v where N_u is the number of vertices of G whose distance to vertex u is smaller than distance to vertex v, and analogously, N_v is the number of vertices of G whose distance to the vertex v
is smaller than to \( u \). The number of vertices equidistant from \( u \) and \( v \) is denoted by \( N_{uv} \). An edge \( uv \) of \( G \) is called a distance-balanced edge if \( N_u = N_v \). A graph \( G \) is said to be distance-balanced \([26]\) if its each edge is distance-balanced. It is known that a connected graph \( G \) is transmission regular if and only if \( G \) is distance balanced \([3], [26]\).

The Szeged index \( Sz(G) \) and the revised Szeged index \( Sz^*(G) \) of a connected graph \( G \) are defined as \([29], [35], [38]\)

\[
Sz(G) = \sum_{uv \in E(G)} N_u N_v, \quad Sz^*(G) = \sum_{uv \in E(G)} \left\{ N_u + \frac{N_{uv}}{2} \right\} \left\{ N_v + \frac{N_{uv}}{2} \right\}.
\]

**Remark 4.** For any connected graph \( G \) with \( n \) vertices, the following known relations are fulfilled \([3], [12], [13], [16], [28], [29], [35], [38], [45]\)

(i) For any edge \( uv \) of \( G \), \( n = N_u + N_v + N_{uv} \). This implies that a graph \( G \) is bipartite if and only if \( n = N_u + N_v \) holds for any edge \( uv \) of \( G \);

(ii) The inequality \( Sz(G) \geq W(G) \) is fulfilled;

(iii) \( Sz(G) \leq Sz^*(G) \) with equality if and only if \( G \) is bipartite;

(iv) For an \( n \)-vertex tree \( T \), \( W(S_n) \leq W(T) \leq W(P_n) \);

(v) For a tree graph \( T \), \( Sz^*(T) = Sz(T) = W(T) \).

The fundamental properties of Wiener index and their extremal graphs are summarized in \([9], [12], [16], [13], [21]\). Transmission regular graphs are characterized by the following property:

**Lemma 5** \([3], [26], [29]\). Let \( G \) be a connected graph with \( n \) vertices and \( m \) edges. Then

\[
Sz^*(G) \leq \frac{n^2 m}{4},
\]
with equality if and only if $G$ is transmission regular.

**Lemma 6** ([3], [12]). Let $G$ be a connected graph and let $uv$ be an edge of $G$. Then

$$\sigma(u) - \sigma(v) = N_v - N_u.$$ 

**Lemma 7.** Let $G$ be a connected graph. Then the following hold:

(i)

$$\text{irr}_T(G) = \sum_{uv \in E(G)} |N_u - N_v| \geq 0;$$

(ii)

$$\sum_{uv \in E(G)} (N_u - N_v)^2 = MSD^2(G) - 2MS^2(G) \geq 0;$$

(iii)

$$\sum_{uv \in E(G)} (\sigma(u) - \sigma(v))^2 = \sum_{uv \in E(G)} (N_u^2 + N_v^2) - 2S_z(G) \geq 0;$$

(iv)

$$\sum_{uv \in E(G)} (N_u^2 + N_v^2) = MSD^2(G) + 2S_z(G) - 2MS^2(G).$$

In (i), (ii) and (iii) the equality holds if and only if $G$ is transmission regular.

**Proof.** (i) is a direct consequence of Lemma 6.
(ii)

\[ 0 \leq \sum_{uv \in E(G)} (N_u - N_v)^2 = \sum_{uv \in E(G)} (\sigma(u) - \sigma(v))^2 = \sum_{uv \in E(G)} (\sigma^2(u) + \sigma^2(v)) - 2 \sum_{uv \in E(G)} \sigma(u)\sigma(v) = \sum_{u \in V(G)} d(u)\sigma^2(u) - 2MS_2(G) \]
\[ = MSD^2_3(G) - 2MS_2(G). \]

(iii)

\[ 0 \leq \sum_{uv \in E(G)} (\sigma(u) - \sigma(v))^2 = \sum_{uv \in E(G)} (N_u - N_v)^2 = \sum_{uv \in E(G)} (N_u^2 + N_v^2) - 2Sz(G). \]

(iv) It follows from the proof of part (ii) and (iii) that

\[ \sum_{uv \in E(G)} (N_u^2 + N_v^2) = \sum_{uv \in E(G)} (\sigma(u) - \sigma(v))^2 + 2Sz(G) = MSD^2_3(G) - 2MS_2(G) + 2Sz(G). \]

\[ \square \]

Remark 5. Based on Lemma 7, the transmission-based topological index \( QS_{v,e}(G) \) can be
represented in the following alternative form:

\[ QS_{v,e}(G) = \frac{n}{2} \left\{ 1 + \frac{1}{m} \sum_{uv \in E(G)} |\sigma(u) - \sigma(v)| \right\} = \frac{n}{2} \left\{ 1 + \frac{1}{m} \sum_{uv \in E(G)} |N_u - N_v| \right\}. \]

**Proposition 5.** Let \( G \) be a connected graph with \( n \) vertices and \( m \) edges. Then

\[ n^2m \geq MSD^3(G) + 4Sz(G) - 2MS_2(G), \]

with equality if and only if \( G \) is a bipartite graph.

**Proof.** Let \( G \) be a connected graph with \( n \) vertices. It follows from Remark 4 (i) that for any edge \( uv \) of \( G \), \( N_u + N_v \leq n \), with equality if and only if \( G \) is bipartite. This implies that

\[ n^2 \geq (N_u + N_v)^2 = (N_u^2 + N_v^2) + 2N_uN_v, \]

with equality if and only if \( G \) is bipartite. Consequently, by Lemma 7 (iv) we have

\[ n^2m = \sum_{uv \in E(G)} n^2 \geq \sum_{uv \in E(G)} (N_u^2 + N_v^2) + 2 \sum_{uv \in E(G)} N_uN_v \]

\[ = \sum_{uv \in E(G)} (N_u^2 + N_v^2) + 2Sz(G) \]

\[ = MSD^3(G) + 4Sz(G) - 2MS_2(G), \]

with equality if and only if \( G \) is bipartite. \( \square \)

**Proposition 6.** Let \( G \) be a connected graph with \( n \) vertices. Then

\[ \text{irr}_{Tr}(G) = \sum_{uv \in E(G)} |N_u - N_v| \geq \frac{1}{n} \sum_{uv \in E(G)} |N_u^2 - N_v^2|, \] (8)
with equality if and only if \( G \) is a bipartite graph.

**Proof.** Let \( G \) be a connected graph with \( n \) vertices. It follows from Remark 4 (i) that for any edge \( uv \) of \( G \), \( N_u + N_v \leq n \), with equality if and only if \( G \) is bipartite. Therefore, it follows from Lemma 6 and

\[
|N_u^2 - N_v^2| = (N_u + N_v)|N_u - N_v| \leq n|N_u - N_v| = n|\sigma(u) - \sigma(v)|,
\]

with equality if and only if \( G \) is bipartite. This implies that Eq. (8) holds with equality if and only if \( G \) is bipartite. \( \square \)

**Corollary 4.** Let \( T_n \) be an \( n \) vertex tree. Then

\[
MS_2(T_n) = 2W(T_n) + \frac{1}{2}MSD^3(T_n) - \frac{n(n - 1)}{2},
\]

\[
\text{irr}_{Tv}(T_n) = \frac{1}{n} \sum_{uv \in E(T_n)} |N_u^2 - N_v^2|.
\]

**Proof.** It is a consequence of Proposition 5, Proposition 6 and Remark 4, since a tree with \( n \) vertices is bipartite and has exactly \( n - 1 \) edges. \( \square \)

**Proposition 7 ( [12]).** Let \( G_B \) be a connected bipartite graph with \( n \) vertices and \( m \) edges. Then

\[
Sz^*(G_B) = Sz(G_B) = \frac{n^2m}{4} - \frac{1}{4} \sum_{uv \in E(G_B)} (\sigma(u) - \sigma(v))^2 \leq \frac{n^2m}{4},
\]

with equality if and only if \( G \) is transmission regular.

**Corollary 5.** Let \( G_B \) be a connected bipartite graph with \( n \) vertices and \( m \) edges. Then

\[
QS_{v,e}(G_B) \leq \sqrt{n^2 - \frac{4}{m}Sz(G_B)},
\]

with equality if and only if \( |\sigma(u) - \sigma(v)| \) is constant for any edge \( uv \in G_B \).
Proof. Using Cauchy-Schwartz inequality and Proposition 7 one obtains for \( G_B \) that

\[
\left\{ \frac{1}{m} \sum_{uv \in E(G_B)} |\sigma(u) - \sigma(v)| \right\}^2 \leq \frac{1}{m} \sum_{uv \in E(G_B)} (\sigma(u) - \sigma(v))^2 = n^2 - \frac{4}{m} Sz(G_B),
\]

with equality if and only if \(|\sigma(u) - \sigma(v)|\) is constant for any edge \( uv \in G_B \). Consequently,

\[
\frac{1}{m} \sum_{uv \in E(G_B)} |\sigma(u) - \sigma(v)| \leq \sqrt{n^2 - \frac{4}{m} Sz(G_B)},
\]

with equality if and only if \(|\sigma(u) - \sigma(v)|\) is constant for any edge \( uv \in G_B \). Because

\[
QS_{v,e}(G_B) - \frac{n}{2} = \frac{n}{2m} \sum_{uv \in E(G_B)} |\sigma(u) - \sigma(v)|,
\]

we have

\[
QS_{v,e}(G_B) - \frac{n}{2} \leq \frac{n}{2} \sqrt{n^2 - \frac{4}{m} Sz(G_B)},
\]

with equality if and only if \(|\sigma(u) - \sigma(v)|\) is constant for any edge \( uv \in G_B \). \( \square \)

Lemma 8 ([12]). Let \( T_n \) be an \( n \)-vertex tree. Then

\[
Sz(T_n) = W(T_n) = \frac{1}{4} \left( n(n - 1) + MS_1(T_n) \right).
\]

The following proposition demonstrates that the Wiener index and the first transmission Zagreb index are closely related.

Proposition 8. Let \( T_n \) be an \( n \)-vertex tree. Then

\[
MS_1(T_n) = 4W(T_n) - n(n - 1) = 4Sz(T_n) - n(n - 1).
\]

(9)
Proof. For any connected graph $G$ we have

$$MS_1(G) = \sum_{uv \in E(G)} (\sigma(u) + \sigma(v)) = \sum_{u \in V(G)} d(u)\sigma(u).$$

Therefore, by Lemma 8 the result follows.

Remark 6. As a consequence of Eq. (9), we conclude that in the family of $n$-vertex trees there is a linear correspondence (a perfect linear correlation) between the topological indices $W(T_n)$ and $MS_1(T_n)$.

In [40] it is reported that for a connected graph $G$, $W(G) < MS_1(G)$. This relation can be strengthened as follows:

Proposition 9. Let $G$ be a connected graph with minimum degree $\delta$ and maximum degree $\Delta$. Then

$$2\delta W(G) \leq MS_1(G) \leq 2\Delta W(G),$$

and equalities hold in both sides if and only if $G$ is a regular graph.

Proof. Because for any connected graph $G$, $MS_1(G) = \sum_{uv \in E(G)} (\sigma(u) + \sigma(v)) = \sum_{u \in V(G)} d(u)\sigma(u)$, and for any vertex $u$ of $G$, $\delta \leq d(u) \leq \Delta$, we have that

$$2\delta W(G) \leq \sum_{uv \in E(G)} (\sigma(u) + \sigma(v)) = \sum_{u \in V(G)} d(u)\sigma(u) \leq 2\Delta W(G).$$

Consequently, if $G$ is an $r$-regular graph, we have $MS_1(G) = 2rW(G)$.

Corollary 6. Let $T_n$ be an $n$-vertex tree. Then

$$(n - 1)(3n - 1) \leq MS_1(T_n) \leq \frac{1}{3}n(n - 1)(2n - 1),$$

where
(i) the right-hand side equality holds if and only if $T_n$ is the path $P_n$;

(ii) the left-hand side equality holds if and only if $T_n$ is the star $S_n$.

Proof. For an $n$-vertex tree $T_n$ we have $W(S_n) \leq W(T_n) \leq W(P_n)$, where $W(S_n) = (n-1)^2$ and $W(P_n) = \frac{(n^3 - n)}{6}$. Therefore, from Proposition 8, we have the following inequalities:

$$MS_1(T_n) \leq \frac{4n(n-1)(n+1)}{6} - n(n-1) = \frac{1}{3}n(n-1)(2n-1),$$

with equality if and only if $T_n$ is the path $P_n$, and

$$MS_1(T_n) \geq 4(n-1)^2 - n(n-1) = (n-1)(3n-1),$$

with equality if and only if $T_n$ is the star $S_n$. \qed

The following is a direct consequence of Proposition 9.

Corollary 7. If $G_{be}$ is a benzenoid graph with $\Delta = 3$ and $\delta = 2$, then

$$4W(G_{be}) \leq MS_1(G_{be}) \leq 6W(G_{be}).$$

It is easy to show that the inequality represented by

$$MS_2(G) = \sum_{uv \in E(G)} \sigma(u)\sigma(v) \leq \frac{1}{2}MSD^3(G),$$

can be sharpened in the following form:

Proposition 10. Let $G$ be a connected graph with $m$ edges. Then

$$MS_2(G) \leq \frac{1}{2}MSD^3(G) - \frac{1}{2m}irr_{Tr}(G)^2,$$
with equality if and only if $|\sigma(u) - \sigma(v)|$ is constant for any $uv \in E(G)$.

**Proof.** Using Cauchy-Schwartz inequality we have

$$\left\{ \frac{1}{m} \sum_{uv \in E(G)} |\sigma(u) - \sigma(v)| \right\}^2 \leq \frac{1}{m} \sum_{uv \in E(G)} (\sigma(u) - \sigma(v))^2,$$

$$= \frac{1}{m} \sum_{uv \in E(G)} (\sigma^2(u) + \sigma^2(v)) - \frac{2}{m} \sum_{uv \in E(G)} \sigma(u)\sigma(v),$$

with equality if and only if $|\sigma(u) - \sigma(v)|$ is constant for any $uv \in E(G)$. It follows that

$$MS_2(G) \leq \frac{1}{2} MSD^3_\infty(G) - \frac{1}{2m} \text{irr}_\text{in}(G)^2,$$

with equality if and only if $|\sigma(u) - \sigma(v)|$ is constant for any $uv \in E(G)$.

**Corollary 8.** Let $G$ be a connected graph with $m$ edges. If $\text{diam}(G) \leq 2$, then

$$MS_2(G) \leq \frac{1}{2} MSD^3_\infty(G) - \frac{1}{2m} \text{irr}(G)^2,$$

with equality if and only if $|d(u) - d(v)|$ is constant for any $uv \in E(G)$.

**Proof.** Let $G$ be a connected graph with $m$ edges. It follows from Remark 3 that for any $uv \in E(G)$, $|d(u) - d(v)|$ is constant if $\text{diam}(G) \leq 2$. Now the result follows from Lemma 3 and Proposition 10.

**Lemma 9 ([41], [14]).** Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$W(G) \geq n(n - 1) - m,$$

with equality if and only if $\text{diam}(G) \leq 2$. (For example, the equality holds for complete graphs, complete bipartite and complete multipartite graphs, moreover wheel graphs and windmill graphs composed of triangles.)
Proposition 11. Let $G$ be a connected $k$-transmission regular with $n$ vertices and $m$ edges. Then

$$k = \frac{2W(G)}{n} \geq 2(n-1) - \frac{2m}{n},$$

with equality if and only if $\text{diam}(G) \leq 2$.

Proof. Since $G$ is $k$-transmission regular, $W(G) = \frac{2k}{n}$. Now the result follows from Lemma 9. \qed

Proposition 12. Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$MS_1^1(G) \geq 4(n-1)W(G) - MS_1^1(G) \geq 4(n-1)(n^2 - n - m) - MS_1(G),$$

and equalities hold in both sides simultaneously if $\text{diam}(G) \leq 2$.

Proof. The result follows directly, using Lemma 9 and Proposition 2. \qed

Proposition 13. Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$MS_1^1(G) \leq \sqrt{m \left\{ MSD_3^2(G) + 2MS_2(G) \right\}},$$

with equality if and only if $\sigma(u) + \sigma(v)$ is constant for each edge $uv \in E(G)$.

Proof. Using the Cauchy-Schwartz inequality, we obtain

$$\left\{ \frac{1}{m} \sum_{uv \in E(G)} (\sigma(u) + \sigma(v)) \right\}^2 \leq \frac{1}{m} \sum_{uv \in E(G)} (\sigma(u) + \sigma(v))^2 \leq \frac{1}{m} \left\{ \sum_{uv \in E(G)} (\sigma^2(u) + \sigma^2(v)) + 2 \sum_{uv \in E(G)} \sigma(u)\sigma(v) \right\},$$

with equality if and only if $\sigma(u) + \sigma(v)$ is constant for each edge $uv \in E(G)$. This implies
that
\[
\left\{ \frac{1}{m} MS_1(G) \right\}^2 \leq \frac{1}{m} \left\{ MSD_{\frac{3}{2}}(G) + 2MS_2(G) \right\},
\]
with equality if and only if \( \sigma(u) + \sigma(v) \) is constant for each edge \( uv \in E(G) \). Consequently, we have
\[
MS_1(G) \leq \sqrt{m \left\{ MSD_{\frac{3}{2}}(G) + 2MS_2(G) \right\}}.
\]

Let \( G \) be a connected graph with \( n \) vertices. Let us define the topological invariant \( \Phi(G) \) as follows
\[
\Phi(G) = \left( \sum_{u \in V(G)} \sigma(u) \right)^2 = \frac{4W(G)^2}{nMS_{\frac{1}{2}}(G)}.
\]

The following theorem shows that \( \Phi(G) \) quantify the degree of transmission regularity of a connected graph \( G \).

**Theorem 1.** Let \( G \) be a connected graph with \( n \) vertices. Then \( \Phi(G) \leq 1 \), with equality if and only if \( G \) is transmission regular.

**Proof.** Using Cauchy-Schwartz inequality, we obtain
\[
\left\{ \sum_{u \in V(G)} \sigma(u) \right\}^2 \leq n \sum_{u \in V(G)} \sigma^2(u),
\]
with equality if and only if \( \sigma(u) = \sigma(v) \) for each \( u, v \in V(G) \). This completes the proof. \( \square \)

**Proposition 14.** Let \( G \) be a connected graph with \( n \) vertices and \( m \)-edges. If \( \rho_D(G) \) denotes the distance spectral radius of \( G \), then
\[
2(n - 1) - \frac{2m}{n} \leq \frac{2W(G)}{n} \leq \rho_D(G).
\]
The left-hand side equality holds if and only if \( \text{diam}(G) \leq 2 \). The right-hand side equality holds if and only if \( G \) is transmission regular.

**Proof.** The left-hand side inequality is noting but Lemma 9. From Theorem 1 and [2, Theorem 5.5] one obtains that
\[
\frac{2W(G)}{n} \leq \sqrt{\frac{1}{n} MS^1(G)} \leq \rho_D(G),
\]
with equality if and only if \( G \) is transmission regular. \( \square \)

Let us finish this section with following result showing how \( W(G), MS_1(G) \) and \( \xi^d(G) \) relates to each other.

**Theorem 2** ([27]). Let \( G \) be a connected graph on \( n \geq 3 \) vertices. Then
\[
MS_1(G) \leq 2nW(G) - \xi^d(G),
\]
with equality if and only if \( G \cong P_4, \) or \( G \cong K_n - ke, \) for \( k = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor \).

### 3 Vertex and edge transitive graphs

In this section, following Darafshe [8], [34], we aim to use a method which applies group theory to graph theory. For more details regarding the theory of groups and graph theory one can see [15] and [19], respectively.

Let \( \Gamma \) be a group acting on a set \( X \). We shall denote the action of \( \alpha \in \Gamma \) on \( x \in X \) by \( x^\alpha \). Then \( U \subseteq X \) is call an orbit of \( \Gamma \) on \( X \) if for every \( x, y \in U \) there exists \( \alpha \in \Gamma \) such that \( x^\alpha = y \). The action of group \( \Gamma \) on \( X \) is called transitive if \( X \) is itself an orbit of \( \Gamma \) on \( X \).

Let \( G \) be a graph. A bijection \( \alpha \) on \( V(G) \) is called an automorphism of \( G \) if it preserves \( E(G) \). In other words, \( \alpha \) is an automorphism if for each \( u, v \in V(G), e = uv \in E(G) \) if and only if \( u^\alpha v^\alpha \in E(G) \). Let us denote by \( Aut(G) \) the set of all automorphisms of \( G \). It is known that \( Aut(G) \) forms a group under the composition of mappings. This is a subgroup of the symmetric group on \( V(G) \). Note that \( Aut(G) \) acts on \( V(G) \) naturally, i.e., for each
\(\alpha \in \text{Aut}(G)\) and \(v \in V(G)\) the action of \(\alpha\) on \(v\), \(v^\alpha\), is defined as \(\alpha(v)\). The action of \(\text{Aut}(G)\) on \(V(G)\) induces an action on \(E(G)\). In fact, for \(\alpha \in \text{Aut}(G)\) and \(e = uv \in E(G)\), the action of \(\alpha\) on \(e = uv\), \(e^\alpha\), is defined as \(u^\alpha v^\alpha\).

A graph \(G\) is called vertex-transitive (edge-transitive) if the action of \(\text{Aut}(G)\) on \(V(G)\) (\(E(G)\)) is transitive.

Let \(G\) be a graph, \(V_1, V_2, \ldots, V_t\) be the orbits of \(\text{Aut}(G)\) under its natural action on \(V(G)\). Then for each \(1 \leq i \leq t\) and for \(u, v \in V_i\), \(\sigma(u) = \sigma(v)\). In particular, if \(G\) is vertex transitive \((t = 1)\), then for each \(u, v \in V(G)\), \(\sigma(u) = \sigma(v)\). Therefore vertex-transitive graphs are transmission regular. It is known that any vertex-transitive graph is (vertex degree) regular \([19]\) and transmission regular \([8]\), but note vise versa.

**Lemma 10.** Let \(G\) be a connected \(k\)-transmission regular graph with \(n\) vertices and \(m\) edges. Then

\[
SJ(G) = \frac{m^2}{(m - n + 2)\sqrt{2k}}, \quad \text{GAS}(G) = \frac{n}{2}, \quad HS(G) = \frac{m}{k},
\]

\[
J(G) = \frac{m^2}{(m - n + 2)k}.
\]

**Lemma 11.** Let \(G\) be a connected vertex-transitive graph with \(n\) vertices and \(m\) edges and the valency \(r\). Then

\[
SJ(G) = \frac{m^2\sqrt{n}}{2(m - n + 2)\sqrt{W(G)}}, \quad \text{GAS}(G) = \frac{2W(G)}{n},
\]

\[
HS(G) = \frac{nm}{2W(G)} = \frac{n^2r}{4W(G)},
\]

\[
J(G) = \frac{m^2n}{2(m - n + 2)W(G)} = \frac{mn^2r}{4(m - n + 2)W(G)}.
\]

**Proof.** If \(G\) is a connected vertex-transitive graph with \(n\) vertices and \(m\) edges, then \(G\) is of valency \(r\) \((r\text{-regular})\) and \(k\)-transmission regular, for some natural numbers \(r\) and \(k\). It follows that \(2m = nr\) and \(2W(G) = nk\). \(\square\)
Lemma 12. Let $G$ be a connected $k$-transmission regular with $n$ vertices and $m$ edges. Then

$$HS(G) \leq \frac{m}{2(n-1)} - \frac{2m}{n},$$

with equality if and only if $\text{diam}(G) \leq 2$.

Proof. Follows from Proposition 11 and the fact that for a $k$-transmission regular graph $G$ with $n$ vertices and $m$ edges, $HS(G) = \frac{m}{k}$. □

Theorem 3. Let $G$ be a connected graph with $n$ vertices and $m$ edges. Let us denote the orbits of the action $\text{Aut}(G)$ on $E(G)$ by $E_1, E_2, \ldots, E_l$. Suppose that for each $1 \leq i \leq t$, $e_i = u_i v_i$ is a fixed edge in the orbit $E_i$. Then

$$HS(G) = \sum_{i=1}^{l} \frac{2|E_i|}{\sigma(u_i) + \sigma(v_i)}, \quad SJ(G) = \frac{m}{m-n+2} \sum_{i=1}^{l} \frac{|E_i|}{\sqrt{\sigma(u_i) + \sigma(v_i)}},$$

$$GAS(G) = \frac{n}{2m} \sum_{i=1}^{l} \frac{|E_i| \sqrt{\sigma(u_i) \sigma(v_i)}}{\sigma(u_i) + \sigma(v_i)}, \quad \text{irr}_T(G) = \sum_{i=1}^{l} |E_i| |\sigma(u_i) - \sigma(v_i)|,$$

$$MS_1(G) = \sum_{i=1}^{l} |E_i| (\sigma(u_i) + \sigma(v_i)), \quad MS_2(G) = \sum_{i=1}^{l} |E_i| \sigma(u_i) \sigma(v_i).$$

Corollary 9. Let $G$ be a connected graph with $n$ vertices and $m$ edges. If $G$ is edge-transitive and $uv$ is a fixed edge of $G$, then

$$HS(G) = \frac{2m}{\sigma(u) + \sigma(v)}, \quad SJ(G) = \frac{m^2}{(m-n+2)\sqrt{\sigma(u) + \sigma(v)}}.$$

$$GAS(G) = \frac{n}{2} \frac{\sqrt{\sigma(u) \sigma(v)}}{\sigma(u) + \sigma(v)}, \quad MS_2(G) = m \sigma(u) \sigma(v)$$

$$\text{irr}_T(G) = m |\sigma(u) - \sigma(v)|, \quad QS_v(G) = |\sigma(u) - \sigma(v)|.$$
\[
Q_{v,e}(G) = \frac{n}{2} \{1 + |\sigma(u) - \sigma(v)|\}, \quad MS_1(G) = m(\sigma(u) + \sigma(v))
\]

Fullerenes are zero-dimensional nanostructures, discovered experimentally in 1985 [30]. Fullerenes \( C_n \) can be drawn for \( n = 20 \) and for all even \( n \geq 24 \). They have \( n \) carbon atoms, \( \frac{3n}{2} \) bonds, 12 pentagonal and \( \frac{n}{2} - 10 \) hexagonal faces. The most important member of the family of fullerenes is \( C_{60} \) [30]. The smallest fullerene is \( C_{20} \). It is a well-known fact that among all fullerene graphs only \( C_{20} \) and \( C_{60} \) (see Figure 3) are vertex-transitive [18]. Since for every vertex of \( v \in V(C_{20}) \), \( \sigma(v) = 50 \) and for every \( v \in V(C_{60}) \), \( \sigma(v) = 278 \), then

\[
SJ(C_{20}) = 7.5, \quad GAS(C_{20}) = 50, \quad HS(C_{20}) = 0.6,
\]

\[
J(C_{20}) = 1.5, \quad SJ(C_{60}) = 10.73, \quad GAS(C_{60}) = 278,
\]

\[
HS(C_{60}) = 0.32, \quad J(C_{60}) = 0.9.
\]

Figure 3: 2-dimensional graph of fullerene \( C_{20} \)

A nanostructure called *achiral polyhex nanotorus* (or *toroidal fullerenes* of parameter \( p \) and length \( q \), denoted by \( T = T[p,q] \) is depicted in Figure 4 and its 2-dimensional molecular graph is in Figure 5. It is regular of valency 3 and has \( pq \) vertices and \( \frac{3pq}{2} \) edges. It follows that
Proposition 15.

\[ SJ(T) = \frac{9(pq)^2 \sqrt{pq}}{8(pq + 2)\sqrt{W(T)}}, \quad GAS(T) = \frac{2W(T)}{pq}, \]

\[ HS(T) = \frac{3(pq)^2}{4W(T)}, \quad J(T) = \frac{9(pq)^3}{8(pq + 2)W(T)}. \]

Figure 4: A achiral polyhex nanotorus (or toroidal fullerene) \( T[p, q] \)

Figure 5: A 2-dimensional lattice for an achiral polyhex nanotorus \( T[p, q] \)

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.

Lemma 13 ( [8]). The hypercube \( H_n \) is \( (n2^{n-1})\)-transmission regular which is vertex- and edge-transitive.

Therefore from Lemma 10 and Lemma 13 we have
Corollary 10.

\[ SJ(H_n) = \frac{n^{2^2(n-1)}}{(n^{2n-1} - 2n + 2)\sqrt{n^{2n}}} \quad \text{GAS}(H_n) = n, \quad HS(H_n) = 2n^{2^2(n-1)}. \]

\[ J(H_n) = \frac{n^{2^2(n-1)}}{(n^{2n-1} - 2n + 2)n^{2n-1}} \]

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