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Wiener–Hosoya Matrix of Connected Graphs

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Abstract: Let \( G \) be a connected (molecular) graph with the vertex set \( V(G) = \{v_1, \cdots, v_n\} \), and let \( d_i \) and \( \sigma_i \) denote, respectively, the vertex degree and the transmission of \( v_i \), for \( 1 \leq i \leq n \). In this paper, we aim to provide a new matrix description of the celebrated Wiener index. In fact, we introduce the Wiener–Hosoya matrix of \( G \), which is defined as the \( n \times n \) matrix whose \((i,j)\)-entry is equal to \( \sigma_i^2 d_i + \sigma_j^2 d_j \) if \( v_i \) and \( v_j \) are adjacent and 0 otherwise. Some properties, including upper and lower bounds for the eigenvalues of the Wiener–Hosoya matrix are obtained and the extremal cases are described. Further, we introduce the energy of this matrix.

Keywords: transmission; vertex-degree; Wiener index; spectral radius, energy

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1. Introduction

Several different topological indices and other molecular descriptors derived from them like energy and spectral radius, have been studied so far and have been used in Quantitative Structure Activity Relationship (QSAR)/Quantitative Structure Property Relationship (QSPR) studies. There exist three wide classes of applicable indices: they are either distance-based, or degree-based or a mixture of them. The first one is defined in terms of distances between pairs of vertices; the second one contains the indices defined as the sums of contributions over all edges.

In this article, we are concerned with the Wiener index which is a most celebrated distance-based topological index, defined as the sum of distances between vertices of a connected graph. The Wiener index of a connected graph was the first topological index to be used in chemistry. It was introduced as the path number of the corresponding graph by Wiener [1], whereby he carried out an investigation into the relationship between the structures and the properties of saturated hydrocarbons. This index is the sum of all shortest carbon–carbon bond paths in a hydrocarbon. This simple numerical representation of a molecule has shown to be a very useful quantity in QSPR. The definition of the Wiener index in terms of distance between vertices of a graph was first given by Haruo Hosoya [2]. In [3] the mathematical aspects of the Wiener index was surveyed.

So far some techniques have been proposed for computing the Wiener index, including the summing up the entries of the Wiener matrix or that of the distance matrix [4,5]. An standard way of computing and describing some specific topological indices is to associate an extended adjacency matrix to them and then investigate the other molecular descriptors derived from them, for example eigenvalues and energy. This technique has been applied to both degree-based (See [6–8] and references therein) and distance-based...
(See [9–14]) topological indices. In the current article, we aim to apply this technique to the celebrated Wiener index.

Throughout of this paper, \( G \) is a simple connected graph with the vertex set \( V(G) = \{v_1, \ldots, v_n\} \) and the edge set \( E(G) \). The degree of a vertex \( v_i \), denoted by \( d_i = d_G(v_i) \), is the number of vertices adjacent to \( v_i \). If the vertices \( v_i \) and \( v_j \) are adjacent, we denote it as \( v_i v_j \in E(G) \) or \( i \sim j \). For any two vertices \( v_i, v_j \in V(G) \), the distance between \( v_i \) and \( v_j \), denoted by \( d_G(v_i, v_j) \), is the number of edges in a shortest path connecting them. The transmission of a vertex \( v_i \in V(G) \), denoted by \( \sigma_i = \sigma_G(v_i) \), is defined as the sum of distances between \( v_i \) and any other vertices in \( G \), i.e.,

\[
\sigma_i = \sigma_G(v_i) = \sum_{j=1}^{n} d_G(v_i, v_j).
\]

The Wiener index of \( G \), denoted by \( W(G) \), has the following representations:

\[
W(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d_G(v_i, v_j) = \frac{1}{2} \sum_{i=1}^{n} \sigma_i = \sum_{i<j} \left( \frac{\sigma_i}{2d_i} + \frac{\sigma_j}{2d_j} \right).
\]

It is obvious that \( \frac{\sigma_i}{2d_i} + \frac{\sigma_j}{2d_j} \) is always positive, and the function

\[
w : E(G) \to \mathbb{R}^+ \quad v_i v_j \mapsto \frac{\sigma_i}{2d_i} + \frac{\sigma_j}{2d_j}
\]

is a weight function on \( E(G) \). We refer to this weight function as the Wiener–Hosoya weighting. Let us denote by \( WH(G) \), the adjacency matrix of \( G \) with respect to the Wiener–Hosoya weighting (2). In fact, \( WH = WH(G) = (w_{i,j}) \), where

\[
w_{i,j} = \begin{cases} \frac{\sigma_i}{2d_i} + \frac{\sigma_j}{2d_j}, & i \sim j; \\ 0, & \text{otherwise}. \end{cases}
\]

Let us name \( WH(G) \) the Wiener–Hosoya matrix of \( G \). Since \( WH(G) \) is symmetric and its diagonal entries are all zero, it follows that

\[
\sum_{1 \leq i,j \leq n} w_{i,j} = 2 \sum_{i=1}^{n} \sum_{j<i} \left( \frac{\sigma_i}{2d_i} + \frac{\sigma_j}{2d_j} \right) = 2 \sum_{j<i} w_{i,j} = 2W(G).
\]

Namely, one half of the sum of all entries of \( WH(G) \) equals the Wiener index of \( G \). Hence, the Wiener–Hosoya matrix provides another way of computing the Wiener index.

Since \( WH(G) \) is real and symmetric, its eigenvalues are all real. Let \( \lambda_1 = \lambda_1(WH(G)) \) denote the \( i \)-th largest eigenvalue of \( WH(G) \), i.e., \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \). We call the eigenvalues of \( WH(G) \), Wiener–Hosoya eigenvalues of \( G \).

Spectral radius of any matrix associated to a (molecular) graph may be used as a molecular descriptor [15–21]. We call the spectral radius of \( WH(G) \), the Wiener–Hosoya spectral radius of \( G \).

The notation of the (adjacency) energy of a graph was introduced by Ivan Gutman in [22] as the sum of absolute values of its adjacency eigenvalues. Since then, this notion was extended to several graph theoretical matrices, especially extended adjacency matrices corresponding to some topological indices [23]. It was also extended to arbitrary non square matrices, [24]. Analogously, we define the Wiener–Hosoya energy of \( G \) as the sum of absolute values of its Wiener–Hosoya eigenvalues, namely
\[ E_{WH}(G) = \sum_{i=1}^{n} |\lambda_i|. \]

In this paper, we aim to obtain some properties, including upper and lower bounds for both the Wiener–Hosoya spectral radius and the Wiener–Hosoya energy of \( G \).

2. Definitions, Notations and Preliminary Results

In this section, we provide more definitions and notations being used hereafter in the present article. Interested readers may refer to [20,25] for more details.

We denote by \( \Delta(G) (\delta(G)) \) the maximum (minimum) vertex degree of \( G \). A graph \( G \) is said to be vertex-degree regular if \( d_G(v_i) = d_G(v_j) \) for each \( v_i, v_j \in V(G) \). A vertex-degree regular graph \( G \) is called \( d \)-vertex-degree regular if \( d_G(v_i) = d \) for each vertex \( v_i \) of \( G \). The maximum (minimum) vertex transmission of \( G \) is denoted by \( \sigma_{\max}(G) (\sigma_{\min}(G)) \). A graph \( G \) is said to be transmission regular [26] if \( \sigma_G(v_i) = \sigma_G(v_j) \) for each \( v_i, v_j \in V(G) \). A transmission regular graph \( G \) is called \( \sigma \)-transmission regular if \( \sigma_G(v_i) = \sigma \) for each vertex \( v_i \) of \( G \). The eccentricity \( \epsilon_G(v_i) \) of a vertex \( v_i \) is the distance between \( v_i \) and a farthest vertex from it, i.e., \( \epsilon_G(v_i) := \max \{d_G(v_i, v_j) \mid v_j \in V(G)\} \). The diameter of \( G \) is defined as the maximum of the eccentricity of its vertices, i.e., \( \text{diam}(G) := \max \{\epsilon_G(v_i) \mid v_i \in V(G)\} \).

Example 1. Let \( G \) be the graph depicted in Figure 1. Then \( G \) is 14-transmission regular, but it is not vertex-degree regular. The Wiener–Hosoya matrix of \( G \) is computed as follows:

\[
\begin{pmatrix}
0 & 14 & 0 & 0 & 0 & 0 & 49 & 49 & 0 \\
14 & 0 & 0 & 0 & 0 & 0 & 49 & 49 & 0 \\
0 & 0 & 14 & 3 & 0 & 0 & 0 & 49 & 0 \\
0 & 0 & 14 & 0 & 0 & 0 & 0 & 49 & 0 \\
0 & 0 & 0 & 0 & 0 & 14 & 49 & 0 & 0 \\
0 & 0 & 0 & 0 & 14 & 0 & 14 & 0 & 14 \\
0 & 0 & 0 & 0 & 0 & 0 & 49 & 0 & 0 \\
14 & 14 & 49 & 0 & 0 & 0 & 0 & 49 & 0 \\
0 & 0 & 14 & 14 & 49 & 0 & 0 & 0 & 0 \\
0 & 0 & 14 & 14 & 49 & 0 & 0 & 0 & 0 \\
0 & 0 & 14 & 14 & 49 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

Note that
\[
d_1 = \cdots = d_6 = 3, \quad d_7 = d_8 = d_9 = 4, \\
w_1 = \cdots = w_6 = \frac{77}{6}, \quad w_7 = w_8 = w_9 = \frac{49}{3}, \\
s_1 = \cdots = s_6 = \frac{35}{3}, \quad s_7 = s_8 = s_9 = \frac{56}{3},
\]

and \( W(G) = 63 \).

![Figure 1](image_url)

Figure 1. A 14-transmission regular graph which is not vertex-degree regular.

The first part of the following lemma proved in [27]; whereas verifying the other parts is straightforward.
Lemma 1. Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then the following hold:
\( (i) \) For any vertex $u \in V(G)$,\[ 2(n - 1) - d_G(u) \leq \sigma_G(u), \]
with equality if and only if $e_G(u) \leq 2$.
\( (ii) \) For any vertex $u$ of $G$, $\sigma_G(u) = 2(n - 1) - d_G(u)$ if and only if $\text{diam}(G) \leq 2$.
\( (iii) \) The following are equivalent whenever $\text{diam}(G) \leq 2$:
\( (a) \) $G$ is transmission regular;
\( (b) \) $G$ is vertex-degree regular;
\( (iv) \) For any vertex $u$ of $G$, $\sigma_G(u) \geq d_G(u)$, with equality if and only if $d_G(u) = n - 1$.
\( (v) \) The ratio of the transmission over the degree of vertices of $G$ is constant if and only if $G$ is both vertex-degree regular and transmission regular.
\( (vi) \) If $\text{diam}(G) \leq 2$, then for any vertex $u$ of $G$, $\sigma_G(u) = \sigma_{\max}(G)$ if and only if $d_G(u) = \delta(G)$.
\( (vii) \)
\[ \frac{\sigma_{\min}(G)}{\Delta(G)} \leq \frac{W(G)}{m} \leq \frac{\sigma_{\max}(G)}{\delta(G)}, \]
with equality if and only if $G$ is both vertex-degree regular and transmission regular.

Lemma 2 ([28,29]). Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then
\[ n(n - 1) - m \leq W(G), \]
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.)

Now let us recall some preliminary results from matrix theory.
A real matrix is called non-negative if its entries are all non-negative. For two real matrices $A$ and $B$ of the same size, we write $A \leq B$ if $B - A$ is non-negative. We write $A < B$, if $A \leq B$ and $A \neq B$. A non-negative matrix $A = (a_{ij})$ is said to be irreducible, if the directed graph $G_A$ with the vertex set $\{1, \ldots, n\}$ and edges $(i, j)$ whenever $a_{ij} > 0$ is strongly connected.

Let $A$ be an arbitrary matrix of size $n \times n$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. The spectrum of $A$, denoted by Spec($A$), is defined as the multi-set of its eigenvalues; we may denote it as
\[ \text{Spec}(A) = \{ \lambda_1^{[m_1]}, \ldots, \lambda_i^{[m_i]} \}, \]
where $\lambda_1, \ldots, \lambda_i$ are the distinct eigenvalues of $A$ with multiplicities $m_1, \ldots, m_i$, respectively. Let us denote the modulus of $\lambda_i$ by $f_i$, for $i = 1, \ldots, n$. The spectral radius (or index) of $A$ is defined as
\[ \rho(A) = \max \{ f_i \mid i = 1, \ldots, n \}. \]
If $A$ is real symmetric, $\lambda_i$’s are all real, and $f_i$’s are nothing but their absolute values.

Lemma 3 (Perron–Frobenius, Symmetric Case [25]). Let $A$ be an $n \times n$, non-negative, symmetric matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then
\( (i) \) $\rho(A) = \lambda_1 \geq -\lambda_n$;
\( (ii) \) If $A$ is irreducible, then $\lambda_1 > \lambda_2$, i.e., $m_1 = 1$;
\( (iii) \) The eigenvalue $\lambda_1$ has a corresponding positive eigenvector.

It is worth noting that Lemma 3 is still valid, if the symmetric assumption is dropped.
Lemma 4 ([30]). Suppose that $A = (a_{ij})$ is an $n \times n$ non-negative matrix with the $i$-th row sum $r_i(A)$, for $i = 1, \ldots, n$. Then
\[
\min_{1 \leq i \leq n} r_i(A) \leq \rho(A) \leq \max_{1 \leq i \leq n} r_i(A).
\] (5)
Besides, the equality on either sides (and hence both sides) of Equation (5) holds if and only if $r_1(A) = \cdots = r_n(A)$.

Lemma 5 ([30]). Let $A$ and $B$ be two square non-negative matrices. If $B$ is irreducible and $A \leq B$, then $\rho(A) \leq \rho(B)$. Especially $\rho(A) < \rho(B)$ if $A < B$.

Lemma 6 (Rayleigh–Ritz [20,25]). Suppose that $A = (a_{ij})$ is an $n \times n$ real, symmetric matrix, with the spectral radius $\lambda_1$. Then for any $x \in \mathbb{R}^n, (x \neq 0)$
\[
x^\top A x \leq \lambda_1 x^\top x.
\]
The equality holds if and only if $x$ is an eigenvector of $A$ corresponding to $\lambda_1$.

3. Relation with Adjacency Matrix

We denote the adjacency matrix of a graph $G$ by $A(G)$. Let us discuss the relationship between $\mathbb{W}(G)$ and $A(G)$ and between their spectrum.

Proposition 1. For a connected graph $G$, we have
\[
\frac{\sigma_{\min}(G)}{\Delta(G)} A(G) \leq \mathbb{W}(G) \leq \frac{\sigma_{\max}(G)}{\delta(G)} A(G),
\]
with equality if and only if $G$ is both vertex-degree regular and transmission regular.

Proof. Let us prove the upper case; The lower case is done analogously. For an arbitrary edge $uv \in E(G)$, we have
\[
\mathbb{W}(G)_{uv} = w(uv) = \frac{\sigma_G(u)}{2d_G(u)} + \frac{\sigma_G(v)}{2d_G(v)} \leq \frac{\sigma_{\max}(G)}{\delta(G)} A(G)_{uv},
\]
from which we have $\mathbb{W}(G) \leq \frac{\sigma_{\max}(G)}{\delta(G)} A(G)$, with equality if and only if $\frac{\mathbb{W}(G)}{|E(G)|} = \frac{\sigma_{\max}(G)}{\delta(G)}$. Hence, by Lemma 1 (vii), we obtain that $\mathbb{W}(G) \leq \frac{\sigma_{\max}(G)}{\delta(G)} A(G)$, with equality if only if $G$ is both vertex-degree regular and transmission regular. \hfill \Box

Let $G$ be a connected graph with $n$ vertices and $\text{diam}(G) \leq 2$. Then it follows from Lemma 1(i) that
\[
\frac{\sigma_{\min}(G)}{\Delta(G)} = \left(\frac{2(n - 1)}{\Delta(G)} - 1\right), \quad \frac{\sigma_{\max}(G)}{\delta(G)} = \left(\frac{2(n - 1)}{\delta(G)} - 1\right).
\]
Hence the following fact follows from Proposition 1 and Lemma 1(ii),(iii).

Corollary 1. Let $G$ be a connected graph with $n$ vertices and $\text{diam}(G) \leq 2$. Then
\[
\left(\frac{2(n - 1)}{\Delta(G)} - 1\right) A(G) \leq \mathbb{W}(G) \leq \left(\frac{2(n - 1)}{\delta(G)} - 1\right) A(G),
\]
with equality if and only if $G$ is vertex-degree regular.
**Remark 1.** Let $G$ be a connected graph which is both $d$-vertex-degree regular and $\sigma$-transmission regular. Then it follows from Proposition 1 that $WH(G) = \frac{\sigma}{d} A(G)$.

Let us finish this section by providing some relations between the Wiener–Hosoya spectrum and the adjacency spectrum of some familiar classes of graphs.

**Example 2.** Let $G$ be a connected graph such that

$$\text{Spec}(A(G)) = \{\alpha_i[m_i], \ldots, \alpha_i[m_t]\}.$$  

If $G$ is both $d$-vertex-degree regular and $\sigma$-transmission regular, then it follows from Remark 1 that

$$\text{Spec}(WH(G)) = \{\frac{\sigma \alpha_i}{d} [m_i], \ldots, \frac{\sigma \alpha_i}{d} [m_t]\}.$$  

A bijection $\theta$ is an automorphism of $G$ if for each $u, v \in V(G)$, $e = uv \in E(G)$ if and only if $e^\theta = u^\theta v^\theta \in E(G)$. A graph $G$ is called vertex-transitive provided that given any two vertices $x$ and $y$ in $V(G)$, there exists an automorphism $\theta$ of $G$ such that $x^\theta = y$. Note that an automorphism of $G$ preserves the distance between vertices of $G$. It is known that a vertex-transitive graph is both vertex-degree regular and transmission regular [25]; however, the converse does not hold in general; For instance, the four-vertex-degree regular graph depicted in Figure 2 is 30-transmission regular graph, but not vertex-transitive, since in a vertex transitive graph, all vertices have equal eccentricities, while in this graph, the eccentricity of vertices is 3 or 4 [31], while in a vertex transitive graph, all vertices have equal eccentricities.

![Figure 2](image1.png)

**Figure 2.** A graph which is both transmission regular and vertex-degree regular, but not vertex-transitive.

**Example 3.** Let $G$ be a connected vertex-transitive graph. Then it is both $d$-vertex-degree regular and $\sigma$-transmission regular. Then by Remark 1, $WH(G) = \frac{\sigma}{d} A(G)$. For instance, let $H$ be the molecular graph of the polyhex nanotorus whose 2-dimensional lattice is depicted in Figure 3. It is cubic, 184-transmission regular, which is vertex-transitive [32]. Therefore $WH(H) = \frac{184}{3} A(H)$.

![Figure 3](image2.png)

**Figure 3.** The 2-dimensional lattice of an achiral polyhex nanotorus (or toroidal fullerene).

**Example 4.** Suppose that $K_n$ denotes the complete graph with $n$ vertices. Then $K_n$ is $(n-1)$-transmission regular, and $(n-1)$-vertex-degree regular. So by Remark 1, $WH(K_n) = A(K_n)$.
Example 5. Let $C_n$ be the cycle graph on $n$ vertices. It is clear that $C_n$ is $\lfloor \frac{n^2}{4} \rfloor$-transmission regular \cite{21}. Hence by Remark 1, $\mathcal{W}(C_n) = \lfloor \frac{n^2}{4} \rfloor \lambda_n(C_n)$.

Example 6. It is well-known that the adjacency eigenvalues of $C_n$ are given by $\alpha_i(C_n) = 2 \cos \frac{2i\pi}{n}$ (see, e.g., \cite{25}). Hence, by Example 2 and Example 5, we have that

\[ \lambda_i(\mathcal{W}(C_n)) = \lfloor \frac{n^2}{4} \rfloor \cos \frac{2i\pi}{n}. \]

By Example 4, the distinct eigenvalues of $\mathcal{W}(K_n)$ are $n-1$ and $-1$, with multiplicities $1$ and $n-1$, respectively, i.e., \(\text{Spec}(\mathcal{W}(K_n)) = \text{Spec}(\Lambda(K_n)) = \left\{(n-1)^{[1]}, -1^{[(n-1)]}\right\}\). 

Example 7. Let $G$ be the graph depicted in Figure 1. Then the characteristic polynomial of $\mathcal{W}(G)$ is as follows:

\[ P_{\mathcal{W}(G)}(x) = x^9 - 3185/12x^7 - 16807/18x^5 + 1289337/64x^3 + 173767573/1296x^2 - 2628866905/10368x^1 + 4747561509943/314928, \]

It follows that

\[ \text{Spec}(\mathcal{W}(G)) = \left\{14.1161^{[1]}, 8.5616^{[2]}, -3.895^{[2]}, -4.6667^{[3]}, -9.4494^{[1]}\right\}. \]

Example 8. Let $F$ be the Fullerene graph depicted in Figure 4. Then the characteristic polynomial of $\mathcal{W}(F)$ is as follows:

\[ P_{\mathcal{W}(F)}(x) = x^{20} - 30x^{18} + 375x^{16} - 24x^{15} - 2540x^{14} + 480x^{13} + 10095x^{12} - 3760x^{11} - 23502x^{10} + 14403x^9 - 28905x^8 - 27000x^7 - 11400x^6 + 20000x^5 - 6000x^4, \]

from which it follows that

\[ \text{Spec}(\mathcal{W}(F)) = \left\{50^{[1]}, 37.2678^{[3]}, 16.6667^{[5]}, 0^{[4]}, -33.3333^{[4]}, -37.2678^{[3]}\right\}. \]
4. Bounds on Wiener–Hosoya Spectral Radius of Connected Graphs

In this section, we study Wiener–Hosoya spectra of connected graphs and establish some (mostly sharp) lower and upper bounds on their elements, and explore the extremal cases. At the end, we present some bonds on the Wiener–Hosoya energy.

Let $G$ be a connected graph. It is easy to verify that $WH(G)$ is irreducible. Furthermore, $WH(G)$ is non-negative. Therefore, the following three results are obtained from Lemma 3, Lemma 4 and Lemma 5, respectively.

**Proposition 2.** Let $G$ be a connected graph on $n$ vertices, let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the Wiener–Hosoya eigenvalues of $G$. Then

(i) $\rho(WH(G)) = \lambda_1 \geq -\lambda_n$;

(ii) $\lambda_1 > \lambda_2$;

(iii) The eigenvalue $\lambda_1$ has a corresponding positive eigenvector.

Before stating the next result, we need to define another notion. We may write $W(G) = \frac{1}{2} \sum_{i=1}^{n} s_i$, where $s_i = \sum_{1 \leq j \leq n} \frac{\sigma_i}{d_j}$. For each $i = 1, 2, \ldots, n$, let $w_i = r_i(WH(G))$ be the $i$-th row sum of $WH(G)$. Namely,

$$w_i = \sum_{1 \leq j \leq n} w_{i,j} = \sum_{1 \leq j \leq n} \left( \frac{\sigma_i}{2d_j} + \frac{\sigma_j}{2d_i} \right) = \frac{1}{2} (\sigma_i + s_i). \quad (7)$$

Note that $w_i$ is the degree of the vertex $v_i$ in the weighted graph $G$ with respect to the Wiener–Hosoya weighting (2). It follows from Equation (4) that

$$2W(G) = \sum_{i=1}^{n} w_i = \frac{1}{2} \sum_{i=1}^{n} (\sigma_i + s_i). \quad (8)$$

Let us call a connected graph $G$, Wiener–Hosoya regular if it is regular graph with respect to the Wiener–Hosoya weighting. Namely, $G$ is Wiener–Hosoya regular if and only if $\sigma_1 + s_1 = \cdots = \sigma_n + s_n$.

**Proposition 3.** Let $G$ be a connected graph on $n$ vertices, and let $\lambda_1$ be the Wiener–Hosoya spectral radius of $G$. Then

$$\min_{1 \leq i \leq n} (\sigma_i + s_i) \leq 2\lambda_1 \leq \max_{1 \leq i \leq n} (\sigma_i + s_i). \quad (9)$$

Equality holds on either side (and hence both sides) of Equation (9) if and only if $G$ is Wiener–Hosoya regular.

Due to the fact that $\frac{1}{2} \min_{1 \leq i \leq n} (\sigma_i + s_i) \leq \frac{2W(G)}{n}$, the following lower bound improves that of Proposition 3.

**Theorem 1.** Let $G$ be a connected graph on $n$ vertices and $m$ edges, and let $\lambda_1$ be the Wiener–Hosoya spectral radius of $G$. Then we have the following:

(i) $$\frac{2W(G)}{n} \leq \lambda_1, \quad (10)$$

with equality if and only if $G$ is Wiener–Hosoya regular.

(ii) $$2(n - 1) - \frac{2m}{n} \leq \lambda_1, \quad (11)$$

with equality if and only if $G$ is Wiener–Hosoya regular and $\text{diam}(G) \leq 2$. 


Proof. (i) Let $x = (x_1, \ldots, x_n)^\top$ be the eigenvector of $\mathcal{WH}(G) = (w_{ij})$ corresponding to $\lambda_1$. By Lemma 6, we obtain that
\begin{equation}
\frac{x^\top \mathcal{WH}(G) x}{x^\top x} = \frac{2 \sum_{i \sim j} w_{ij} x_i x_j}{\sum_{i=1}^n x_i^2} \leq \lambda_1.
\end{equation}
Since the vector $x$ in Equation (12) is arbitrary taken, by putting $x = \frac{1}{\sqrt{n}} (1, 1, \ldots, 1)^\top$, and keeping in mind Equation (4), we arrive at
\begin{equation}
\frac{2W(G)}{n} = \frac{2 \sum_{i \sim j} w_{ij}}{n} \leq \lambda_1.
\end{equation}
Now, let us discuss the equality case in Equation (10). Suppose that $G$ is Wiener–Hosoya regular such that $w = \sigma_1 + s_1 = \cdots = \sigma_n + s_n$. Then by Proposition 3, $2\lambda_1 = w$. Thus by Equation (8), we obtain that $\lambda_1 = \frac{2W(G)}{n}$ and hence the equality holds in Equation (10). Conversely, if the equality holds in Equation (10), then
\begin{equation}
2n\lambda_1 = 2W(G) = \sum_{i=1}^n w_i = \sum_{i=1}^n (\sigma_i + s_i),
\end{equation}
from which we obtain that
\begin{equation}
2\lambda_1 = (\sigma_i + s_i), \quad 1 \leq i \leq n,
\end{equation}
showing that $G$ is Wiener–Hosoya regular.

(ii) This part is a direct consequence of (i) and Lemma 2. □

The following two results are direct consequences of Proposition 1 and Corollary 1, respectively.

Proposition 4. Let $G$ be a connected graph, and let $\lambda_1$ and $\alpha_1$ be, respectively, the Wiener–Hosoya spectral radius and the (adjacency) spectral of $G$. Then
\[
\frac{\sigma_{\min}(G)}{\Delta(G)} \alpha_1 \leq \lambda_1 \leq \frac{\sigma_{\max}(G)}{\delta(G)} \alpha_1.
\]
Besides the equality holds if and only if $G$ is both vertex-degree regular and transmission regular.

Corollary 2. Let $G$ be a connected graph with $n$ vertices and $\text{diam}(G) \leq 2$. If $\lambda_1$ is the Wiener–Hosoya spectral radius of $G$, then
\[
\left( \frac{2(n-1)}{\Delta(G)} - 1 \right) \alpha_1 \leq \lambda_1 \leq \left( \frac{2(n-1)}{\delta(G)} - 1 \right) \alpha_1.
\]
Besides the equality holds if and only if $G$ is vertex-degree regular.

With the aim of the following result, we may obtain bounds for the roots of graph polynomials.

Lemma 7 ([33]). For real numbers $c_1$ and $c_2$, we denote $\Psi_n(c_1, c_2)$ as the set of monic, real polynomials of degree $n$ and of the form
\[
P_n(\lambda) = \lambda^n + c_1 \lambda^{n-1} + c_2 \lambda^{n-2} + b_3 \lambda^{n-3} + \cdots + b_n.
\]
Suppose that \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \) are the roots of \( P_n(\lambda) \in \mathcal{P}_n(c_1,c_2) \), i.e., \( P_n(\lambda) = \prod_{i=1}^{n} (\lambda - \lambda_i) \). Then

\[
\lambda + \frac{1}{n} \sqrt{\frac{\Delta}{n-1}} \leq \lambda_1 \leq \lambda + \frac{1}{n} \sqrt{\Delta(n-1)}, \quad (16)
\]

\[
\lambda - \frac{1}{n} \sqrt{\frac{\Delta(i-1)}{n-i+1}} \leq \lambda_i \leq \lambda - \frac{1}{n} \sqrt{\Delta(n-i)}, \quad i = 2,3,\ldots,n-1
\]

where

\[
\lambda = \frac{1}{n} \sum_{i=1}^{n} \lambda_i = -\frac{c_1}{n} \quad \text{and} \quad \Delta = n \sum_{i=1}^{n} \lambda_i^2 - \left( \sum_{i=1}^{n} \lambda_i \right)^2,
\]

\[
c_2 = \frac{1}{2} \left( \left( \sum_{i=1}^{n} \lambda_i \right)^2 - \sum_{i=1}^{n} \lambda_i^2 \right) = \frac{1}{2} \left( n\lambda^2 - \sum_{i=1}^{n} \lambda_i^2 \right).
\]

**Theorem 2.** Let \( G \) be a connected graph on \( n \) vertices, and let \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \) be the Wiener–Hosoya eigenvalues of \( G \). Then

\[
\frac{1}{n} \sqrt{\frac{n \text{tr}(WH^2)}{n-1}} \leq \lambda_1 \leq \frac{1}{n} \sqrt{n(n-1) \text{tr}(WH^2)} \quad (19)
\]

\[
\frac{1}{n} \sqrt{\frac{(i-1)n \text{tr}(WH^2)}{n-i+1}} \leq \lambda_i \leq \frac{1}{n} \sqrt{n(n-i) \text{tr}(WH^2)} \quad \text{for } i = 2, \ldots, n-1
\]

\[
\frac{1}{n} \sqrt{n(n-1) \text{tr}(WH^2)} \leq \lambda_n \leq \frac{1}{n} \sqrt{n \text{tr}(WH^2) \cdot n-1}.
\]

**Proof.** If \( P_{WH(G)}(\lambda) \) is the characteristic polynomial of \( WH(G) \), then

\[
P_{WH(G)}(\lambda) = \prod_{i=1}^{n} (\lambda - \lambda_i) = \lambda^n + c_1 \lambda^{n-1} + c_2 \lambda^{n-2} + b_3 \lambda^{n-3} + \cdots + b_n,
\]

where it follows from the properties of the coefficients of characteristic polynomials,

\[
c_1 = -\sum_{i=1}^{n} \lambda_i = -\text{tr}(WH(G)) = 0,
\]

and

\[
c_2 = \sum_{1 \leq i < j \leq n} \lambda_i \lambda_j = \frac{1}{2} \left( \left( \sum_{i=1}^{n} \lambda_i \right)^2 - \sum_{i=1}^{n} \lambda_i^2 \right) = \frac{1}{2} (-\text{tr}(WH^2)).
\]

Hence \( P_{WH(G)}(\lambda) \in \mathcal{P}_n(0,\frac{1}{2}(-\text{tr}(WH^2))) \), and therefore by Lemma 7, the results hold. \( \square \)

Now let us finish this article by expressing the following result:

**Proposition 5.** The following inequalities hold for \( \lambda_1 = f_1 \geq f_2 \geq \cdots \geq f_n \):

\[
\frac{E_{WH}}{n} + \frac{1}{n} \sqrt{\frac{n \text{tr}(WH^2)}{n-1} - E_{WH}^2} \leq f_1 \leq \frac{E_{WH}}{n} + \frac{1}{n} \sqrt{(n-1) \text{tr}(WH^2) - E_{WH}^2}, \quad (20)
\]
\[ \begin{align*}
\mathcal{E}_{WH} & - \frac{1}{n} \sqrt{\frac{(i - 1)(n \text{ tr}(WH^2) - \mathcal{E}_{WH}^2)}{n - i + 1}} \leq f_i \\
& \leq \frac{1}{n} \sqrt{\frac{(n - i)(n \text{ tr}(WH^2) - \mathcal{E}_{WH}^2)}{i}}, \quad i = 2, \ldots, n - 1,
\end{align*} \]

(21)

\[ \begin{align*}
\mathcal{E}_{WH} & - \frac{1}{n} \sqrt{(n - 1)(n \text{ tr}(WH^2) - \mathcal{E}_{WH}^2)} \leq f_u \leq \frac{1}{n} \sqrt{n \text{ tr}(WH^2) - \mathcal{E}_{WH}^2} \\
& \leq \frac{1}{n} \sqrt{\frac{n \text{ tr}(WH^2) - \mathcal{E}_{WH}^2}{n - 1}}
\end{align*} \]

(22)

Proof. Consider the polynomial

\[ P_n(\lambda) = \prod_{i=1}^{n} (\lambda - f_i) = \lambda^n + c_1 \lambda^{n-1} + c_2 \lambda^{n-2} + b_3 \lambda^{n-3} + \cdots + b_n. \]

Since

\[ c_1 = - \sum_{i=1}^{n} f_i = -\mathcal{E}_{WH} \]

and

\[ c_2 = \frac{1}{2} \left( \left( \sum_{i=1}^{n} f_i \right)^2 - \sum_{i=1}^{n} f_i^2 \right) = \frac{1}{2} (\mathcal{E}_{WH}^2 - \text{tr}(WH^2)), \]

the polynomial \( P_n(\lambda) \) belongs \( \psi_n \left( -\mathcal{E}_{WH}, \frac{1}{2} \mathcal{E}_{WH}^2 - \frac{1}{2} \text{tr}(W^2) \right) \). Now, based on Equation (17) we have that

\[ \lambda = \frac{1}{n} \sum_{i=1}^{n} f_i = \frac{\mathcal{E}_{WH}}{n}, \]

\[ \Delta = n \sum_{i=1}^{n} f_i^2 - \left( \sum_{i=1}^{n} f_i \right)^2 = n \text{ tr}(WH^2) - \mathcal{E}_{WH}^2. \]

By substituting \( \Delta \) and \( \bar{\lambda} \) in Equation (16), the required inequalities are obtained. \( \square \)

5. Concluding Remarks

In mathematical chemistry, studying the upper and lower bounds of a molecular descriptor are important due to the fact that they provide some useful information to approximate the range of the applicability of the descriptor in QSAR and QSAR in terms of structural parameters of a molecule (graph). In this article, we introduce the Wiener–Hosoya matrix, which is an extended adjacency matrix of the Wiener index and then, we establish some upper and lower bond for its spectral radius and its energy.

It is worth noting that the techniques in this report are naturally extended to other Wiener like topological indices, like the Harary index, the reciprocal reverse Wiener index, the reciprocal complementary Wiener index, the Kirchhoff index and the detour index.

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