Hosoya polynomial of composite graphs

Dragan Stevanović
Department of Mathematics, Faculty of Philosophy,
Čirila i Metodija 2, Niš 18000, Yugoslavia
dragance@filfak.filfak.ni.ac.yu

Abstract
Let $G_1 + G_2$, $G_1 \bigtriangleup G_2$, $G_1 \bigcirc G_2$, $G_1 \circ G_2$ and $G_1 \{G_2\}$ be the sum, join, composition, corona and cluster, respectively, of the graphs $G_1$ and $G_2$. Elsewhere, Yeh and Gutman computed the Wiener number of these composite graphs. In this paper, we generalize their results to compute the Hosoya polynomial of these graphs.

1 Introduction
In this paper, we are concerned with finite undirected graphs without loops or multiple edges. If $G$ is such a graph, denote its vertex- and edge-sets with $V(G)$ and $E(G)$, respectively. If $v$ is a vertex of $G$ we write shortly $v \in G$. The numbers of vertices and edges of $G$ will be denoted by $|G|$ and $|E(G)|$, respectively.

Let $d(u, v \mid G)$ be the distance between the vertices $u$ and $v$ of a connected graph $G$. Define

\begin{align*}
W(G) & = \frac{1}{2} \sum \{d(u, v \mid G) : u, v \in G\} \\
H(G, x) & = \frac{1}{2} \sum \{x^{d(u, v \mid G)} : u, v \in G, u \neq v\}.
\end{align*}

Hence, $W(G)$ is just the sum of distances between all pairs of vertices of $G$. The investigation of the quantity $W(G)$ seems to be first undertaken by Harold Wiener [23] over 50 years ago, in connection with certain chemical applications. More details on usages of $W(G)$ in chemistry can be found in [12], or more recent surveys [13, 20]. The name Wiener number or Wiener index is nowadays in standard use in chemistry and is sometimes encountered also in the mathematical literature [16, 17, 18].

Wiener’s original article [23] appeared in a chemistry journal and was long overlooked by mathematicians. The Wiener number is first considered in the mathematical literature (under the name graph distance) in the seventies by Entringer, Jackson and Snyder [6]. Since then, it has been extensively studied...
in graph theory (see [2]), and a variety of names was proposed for it: gross status [14], total status [2], graph distance [6], transmission [21, 22], and simply sum of all distances [25, 8]. In some papers, closely related mean distance [5, 24] or average distance [1, 3] were considered.

The polynomial $H(G, x)$ is named the Wiener polynomial in [15], but we call it the Hosoya polynomial in honor of Haruo Hosoya, who introduced it in [15]. This name is also used in [19, 10]. The Hosoya polynomial is more recent notion generalizing the Wiener number. Notice that

$$(3) \quad H(G, 1) = \left(\frac{|G|}{2}\right), \quad H'(G, 1) = W(G).$$

A reason more for considering Hosoya polynomial is that it can be differentiated several times. Let $H^{(k)}(G, x)$ be the $k^{th}$ derivative of the Hosoya polynomial with respect to $x$. The quantities $W^{(k)}(G) = H^{(k)}(G, 1)$, $k \geq 2$, may be viewed as the higher Wiener numbers. They are recently shown to have some significance in the studies of organic compounds [7].

### 2 Hosoya polynomial of composite graphs

Yeh and Gutman [25] examined the Wiener number in the case of graphs that are obtained by means of certain binary operations on pairs of graphs. They considered the following composite graphs:

(a) The sum $G_1 + G_2$ (called product and denoted by $G_1 \times G_2$ in [25]):

$$V(G_1 + G_2) = V(G_1) \times V(G_2);$$

the vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $G_1 + G_2$ are adjacent iff $[u_1 = v_1, (u_2, v_2) \in E(G_2)]$ or $[u_2 = v_2, (u_1, v_1) \in E(G_1)]$.

(b) The join $G_1 \bigtriangledown G_2$ (denoted by $G_1 + G_2$ in [25]):

$$V(G_1 \bigtriangledown G_2) = V(G_1) \cup V(G_2);$$

$$E(G_1 \bigtriangledown G_2) = E(G_1) \cup E(G_2) \cup \{(u_1, u_2) | u_1 \in G_1, u_2 \in G_2\}.$$

(c) The composition $G_1 [G_2]$:

$$V(G_1 [G_2]) = V(G_1) \times V(G_2);$$

the vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $G_1 [G_2]$ are adjacent iff $[u_1 = v_1, (u_2, v_2) \in E(G_2)]$ or $[u_2 = v_2, (u_1, v_1) \in E(G_1)]$.

(d) The corona $G_1 \circ G_2$ is obtained by taking one copy of $G_1$ and $|G_1|$ copies of $G_2$, and by joining each vertex of the $i^{th}$ copy of $G_2$ to the $i^{th}$ vertex of $G_1$, $i = 1, 2, \ldots, |G_1|$.
The cluster \( G_1 \{ G_2 \} \) is obtained by taking one copy of \( G_1 \) and \(|G_1|\) copies of a rooted graph \( G_2 \), and by identifying the root of the \( i \)th copy of \( G_2 \) with the \( i \)th vertex of \( G_1 \), \( i = 1, 2, \ldots, |G_1| \).

Theorems 1–5 dealing with the Hosoya polynomial of composite graphs generalize the Theorems 1–5 proved in [25] for the Wiener number. From now on, we shortly write \( H(G) \) instead of \( H(G, x) \).

**Theorem 1** For any two graphs \( G_1 \) and \( G_2 \),

\[
H(G_1 + G_2) = 2H(G_1)H(G_2) + |G_1|H(G_2) + |G_2|H(G_1).
\]

**Theorem 2** For any two graphs \( G_1 \) and \( G_2 \),

\[
H(G_1 \nabla G_2) = \left[ \binom{|G_1|}{2} + \binom{|G_2|}{2} \right] x^2 - \left[ |E(G_1)| + |E(G_2)| \right] x(x-1) + |G_1||G_2| x.
\]

**Theorem 3** For any two graphs \( G_1 \) and \( G_2 \),

\[
H(G_1 [G_2]) = |G_2|^2 H(G_1) + |G_1| \binom{|G_2|}{2} x^2 - |G_1||E(G_2)| x(x-1).
\]

**Theorem 4** For any two graphs \( G_1 \) and \( G_2 \),

\[
H(G_1 \circ G_2) = (1 + |G_2| x)^2 H(G_1) + |G_1| \left[ \binom{|G_2|}{2} - |E(G_2)| \right] x^2 + |G_1||G_2| + |E(G_2)| x.
\]

**Theorem 5** Let \( G_2 \) be connected graph with root-vertex \( r \). Then,

\[
H(G_1 \{ G_2 \}) = H_0(r, G_2)^2 H(G_1) + |G_1| H(G_2),
\]

where \( H_0(r, G) = \sum_{u \in G} x^{d(r, u)} \).

Notice that the results from [25] hold only for connected graphs. From that reason it is defined there that \( W(G) = \infty \) for disconnected graphs. More natural approach is to define both the Wiener number and the Hosoya polynomial of disconnected graphs component-wise:

- if \( G \) has the components \( G_i \) \( (i = 1, \ldots, c(G)) \),
  - then \( W(G) = \sum_i W(G_i) \) and \( H(G, x) = \sum_i H(G_i, x) \).

Since the equations (4)-(8) hold for disconnected graphs, the Wiener number of disconnected composite graphs may be obtained by differentiating the Hosoya polynomial.
3 Proofs

We prove the Theorems 1–5 only for connected graphs. The step from the connected graphs to disconnected ones is done using the following consideration. Suppose the components of $G_1$ are $G_{1,i}$ ($i = 1, \ldots, c(G_1)$), while those of $G_2$ are $G_{2,j}$ ($j = 1, \ldots, c(G_2)$). Then $G_1 + G_2$ has components $G_{1,i} + G_{2,j}$ ($i = 1, \ldots, c(G_1); j = 1, \ldots, c(G_2)$), and

$$H(G_1 + G_2) = H\left(\bigcup_i \bigcup_j G_{1,i} + G_{2,j}\right) = \sum_i \sum_j H(G_{1,i} + G_{2,j})$$

$$= \sum_i \sum_j \left(2H(G_{1,i})H(G_{2,j}) + |G_{1,i}|H(G_{2,j}) + |G_{2,j}|H(G_{1,i})\right)$$

$$= 2 \sum_i H(G_{1,i}) \sum_j H(G_{2,j}) + \sum_i |G_{1,i}| \sum_j H(G_{2,j}) + \sum_j |G_{2,j}| \sum_i H(G_{1,i})$$

$$= 2H(G_1)H(G_2) + |G_1|H(G_2) + |G_2|H(G_1).$$

This way the formula which holds for the sum of connected graphs extends to the sum of disconnected ones. Similar proofs hold in other cases.

**Proof of Theorem 1.** Consider two distinct vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ in $G_1 + G_2$. As in [25], we first show that

$$d(u, v \mid G_1 + G_2) = d(u_1, v_1 \mid G_1) + d(u_2, v_2 \mid G_2).$$

Let $d(u_j, v_j \mid G_j) = d_j$ ($j = 1, 2$). Let

$$u = (p_0, p_1, p_2), \ldots, (p_{k-1}, p_k), (p_1, p_2) = v$$

be the shortest path in $G_1 + G_2$ between $u$ and $v$. Then for $i$ ($0 \leq i \leq k - 1$) holds either that $[p_i, p_{i+1}]$ is adjacent to $p_i^1$, $p_i^2$, $p_{i+1}^1$, $p_{i+1}^2$ or that $p_i^1 = p_i^2$ holds. Let $S_j$ denote the number of vertex-pairs $p_i^1, p_{i+1}^1$ for which $p_i^1 \neq p_{i+1}^1$ ($i = 0, 1, \ldots, k - 1; j = 1, 2$). From above follows $S_1 + S_2 = k$, and since $S_j \geq d_j$ ($j = 1, 2$) we conclude that $d(u, v \mid G_1 + G_2) = k \geq d_1 + d_2$.

On the other hand, let $u_j = q_0^j, q_1^j, \ldots, q_{d_j}^j = v_j$ be the shortest path between $u_j$ and $v_j$ in $G_j$ ($j = 1, 2$). Then the following path in $G_1 + G_2$ between $u$ and $v$

$$(u_1, u_2) = (q_0^1, q_0^2), (q_1^1, q_0^2), \ldots, (q_{d_1}^1, q_0^2), (q_1^2, q_1^2), \ldots, (q_{d_1}^2, q_{d_2}^2) = (v_1, v_2)$$

has the length $d_1 + d_2$ and so $d(u, v \mid G_1 + G_2) = d_1 + d_2$. Now,

$$H(G_1 + G_2) = \frac{1}{2} \sum \{x^{d(u,v \mid G_1 + G_2)} : u, v \in G_1 + G_2, u \neq v\}$$

$$= \frac{1}{2} \sum \{x^{d(u_1, v_1 \mid G_1)}x^{d(u_2, v_2 \mid G_2)} : u_1, v_1 \in G_1, u_2, v_2 \in G_2, u_1 \neq v_1 \lor u_2 \neq v_2\}$$

$$= \frac{1}{2} \sum \{x^{d(u_1, v_1 \mid G_1)}x^{d(u_2, v_2 \mid G_2)} : u_1 \neq v_1, u_2 \neq v_2\}$$

4
graphs with roots general result. Let $G$

Proof of Theorem 3. Consider two vertices $G$

Proof of Theorem 2. Any two vertices of $G_1 \vee G_2$ are either adjacent or at distance two. The distance-two pairs are those corresponding to nonadjacent vertices in either $G_1$ or $G_2$. Hence,

$$H(G_1 \vee G_2) = \left[ \left( \frac{|G_1|}{2} \right) - |E(G_1)| + \left( \frac{|G_2|}{2} \right) - |E(G_2)| \right] x^2 + \left[ |E(G_1)| + |E(G_2)| + |G_1||G_2| \right] x,$$

and we arrive at (5). ■

Proof of Theorem 3. Consider two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $G_1[G_2]$. Note that

$$d(u, v | G_1[G_2]) = \begin{cases} d(u_1, v_1 | G_1), & \text{if } u_1 \neq v_1 \\ 1, & u_1 = v_1 \text{ and } (u_2, v_2) \in E(G_2) \\ 2, & u_1 = v_1 \text{ and } (u_2, v_2) \notin E(G_2). \end{cases}$$

Hence,

$$H(G_1[G_2]) = \frac{1}{2} \sum \{ x^{d(u,v | G_1[G_2])} : u, v \in G_1[G_2], u \neq v \}$$

$$= \frac{1}{2} \sum \{ x^{d(u_1,v_1 | G_1)} : u_1, v_1 \in G_1, u_2, v_2 \in G_2, u_1 \neq v_1 \}$$

$$+ \frac{1}{2} \sum \{ x^2 : u_1 = v_1, (u_2, v_2) \notin E(G_2) \}$$

$$+ \frac{1}{2} \sum \{ x : u_1 = v_1, (u_2, v_2) \in E(G_2) \}$$

$$= |G_2|^2 H(G_1) + |G_1| \left( \left( \frac{|G_2|}{2} \right) - |E(G_2)| \right) x^2 + |G_1||E(G_2)| x.$$ ■

Before we give the proofs of Theorems 4 and 5, we prove a slightly more general result. Let $G$ be any graph and $R_1, R_2, \ldots, R_{|G|}$ be rooted connected graphs with roots $r_1, r_2, \ldots, r_{|G|}$, respectively. The graph $G[R_1, R_2, \ldots, R_{|G|}]$ is obtained by identifying the root $r_i$ of $R_i$ with the $i^{th}$ vertex of $G$. It holds

$$H(G[R_1, R_2, \ldots, R_{|G|}]) = \sum_{1 \leq i \leq |G|} H(R_i) + \sum_{1 \leq i < j \leq |G|} H_0(r_i, R_i) H_0(r_j, R_j) x^{d(i,j | G)}.$$

(9) $H(G[R_1, R_2, \ldots, R_{|G|}]) = \sum_{1 \leq i \leq |G|} H(R_i) + \sum_{1 \leq i < j \leq |G|} H_0(r_i, R_i) H_0(r_j, R_j) x^{d(i,j | G)}$.  

5
If two distinct vertices \(u, v\) belong to the same \(R_i\), then
\[
d(u, v \mid G\{R_1, R_2, \ldots, R_{|G|}\}) = d(u, v \mid R_i),
\]
and summing up terms \(x^{d(u, v \mid R_i)}\) for all unordered pairs of distinct vertices from the same \(R_i\) we get the term \(\sum_{1 \leq i \leq |G|} H(R_i)\) from (9).

If \(u\) belong to \(R_i\) and \(v\) belong to \(R_j\) with \(i \neq j\), then
\[
d(u, v \mid G\{R_1, R_2, \ldots, R_{|G|}\}) = d(u, r_i \mid R_i) + d(i, j \mid G) + d(r_j, v \mid R_j),
\]
and so
\[
x^{d(u, v \mid G\{R_1, R_2, \ldots, R_{|G|}\})} = x^{d(u, r_i \mid R_i)} x^{d(i, j \mid G)} x^{d(r_j, v \mid R_j)}.
\]
Summing up terms \(x^{d(u, r_i \mid R_i)} x^{d(i, j \mid G)} x^{d(r_j, v \mid R_j)}\) for all unordered pairs of vertices from distinct \(R_i\)'s we get term \(\sum_{1 \leq i < j \leq |G|} H_0(r_i, R_i) H_0(r_j, R_j) x^{d(i, j \mid G)}\) from (9).

**Proof of Theorem 5.** This theorem follows directly from (9) since we have that \(G_1 \{G_2\} = G_1 \{G_2, G_2, \ldots, G_2\}\). ■

**Proof of Theorem 4.** Theorem 4 is a special case of Theorem 5. We have \(G_1 \circ G_2 \equiv G_1 \{G_2 \nabla K_1\}\), where \(K_1\) is the one-vertex graph and where the root of \(G_2 \nabla K_1\) is chosen to be the vertex of \(K_1\). ■

### 4 Examples

In this section we report the Hosoya polynomials of several classes of composite graphs, that can be obtained from simple graphs by applying the operations considered. Let \(S_n, P_n, C_n\) and \(K_n\) denote the star, path, cycle and complete graph, respectively, on \(n\) vertices. Further, let \(\overline{G}\) be the complement of \(G\), and let \(t = \frac{x}{x-1}\). A simple calculation gives:

\[
H(S_n) = \left(\frac{n-1}{2}\right) x^2 + (n-1)x,
\]
\[
H(P_n) = x^{n-1} + 2x^{n-2} + \ldots + (n-1)x = (x^{n-1} - 1) t^2 - (n-1) t,
\]
\[
H(C_n) = nx^{n/2} + nx^{n/2-1} + \ldots + nx = n x^{n/2}(t - t), \text{ for } n \text{ odd},
\]
\[
= \frac{n}{2} x^{n/2} + nx^{n/2-1} + \ldots + nx = n x^{n/2}(t - \frac{1}{2} t), \text{ for } n \text{ even}.
\]

The complete multipartite graph \(K_{a_1, a_2, \ldots, a_p}\), \(p > 1\), on \(a_1 + a_2 + \ldots + a_p = n\) vertices is presented as \(K_{a_1} \nabla K_{a_2} \nabla \ldots \nabla K_{a_p}\), which yields
\[
H(K_{a_1, a_2, \ldots, a_p}) = \sum_i \left(\frac{a_i}{2}\right) x^2 + \prod_{i<j} a_i a_j x.
\]
The graphs \( Grd_{m,n} = P_m + P_n \), \( Sun_{m,n} = C_m \{ P_{n+1} \} \) and \( Whl_{m,n} = \overline{K}_m \nabla C_n \) are called the grid, sun and generalized wheel, respectively. In the case of sun it is assumed that \( P_{n+1} \) is rooted at vertex of degree one. The Hosoya polynomials are given by

\[
H(Grd_{m,n}) = 2 (x^{m-1} - 1)(x^{n-1} - 1) t^4 \\
-2 \left( (m - 1)x^{n-1} + (n - 1)x^{m-1} - m - n + 2 \right) t^3 \\
+ \left( 2 (m - 1)(n - 1) + mx^{n-1} + nx^{m-1} - m - n \right) t^2 \\
- \left( 2 (m - 1)(n - 1) + m + n - 2 \right) t,
\]

\[
H(Grd_{n,n}) = 2 (x^{n-1} - 1)^2 t^4 - 2 (x^{n-1} - 1)(2nt - 2t - n) t^2 \\
+2 (n - 1) t (nt - t - n), \text{ for the square grid (} m = n \text{)},
\]

\[
H(Whl_{m,n}) = \frac{n(n-3) + m(m-1)}{2} x^2 + n(m+1)x,
\]

\[
H(Whl_{1,n}) = \frac{n(n-3)}{2} x^2 + 2nx, \text{ for the simple wheel (} m = 1 \text{)},
\]

\[
H(Sun_{m,n}) = m \left( x^{[m/2]} t - t \right) \left( \frac{x^{n+1}}{x-1} \right)^2 + m \left( x^n t^2 - nt \right), \text{ if } m \text{ is odd},
\]

\[
= m \left( x^{[m/2]} \left( t - \frac{1}{2} \right) - t \right) \left( \frac{x^{n+1}}{x-1} \right)^2 + m \left( x^n t^2 - nt \right), \text{ if } m \text{ is even}.
\]

The \( r \)-fold bristled graph of \( G \), denoted by \( Brs_r(G) \), is defined as \( G \{ S_{r+1} \} \) where the root of \( S_{r+1} \) is on its vertex of degree \( r \). Then

\[
H(Brs_r(G)) = (1 + rx)H(G) + \left[ \left( \frac{r}{2} \right) x^2 + rx \right] |G|.
\]

For the simple bristled graph \( (r = 1) \),

\[
H(Brs_1(G)) = (1 + x)H(G) + x|G|.
\]

References


