

HOSOYA POLYNOMIAL OF THORN TREES, RODS, RINGS, AND STARS

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ABSTRACT. The Hosoya polynomial is determined for thorn trees, thorn rods, rings, and stars, which are special cases of thorn graphs. By this some earlier results by Bonchev and Klein are generalized. Various distance-based topological indices, namely Wiener index, hyper-Wiener index, Harary index, and reciprocal Wiener index can thus be computed for the classes of graphs under consideration.

INTRODUCTION: DISTANCE-BASED MOLECULAR STRUCTURE-DESCRIPTORS

The Wiener index is a graph invariant of great chemical importance. It is defined as

$$W = W(G) = \sum_{u < v} d(u, v) \quad (1)$$

where G is the graph representation of the molecule under consideration and $d(u, v)$ is the distance between the vertices u and v of G . On the numerous chemical applications of the Wiener index see the reviews [1–4] and the references quoted therein; on its mathematical properties see the reviews [5,6].

Recently several modifications of the Wiener index were put forward, of which we mention the following:

the hyper–Wiener index [7–10]:

$$WW = WW(G) = \frac{1}{2} \sum_{u < v} [d(u, v)^2 + d(uv)] \quad (2)$$

the Harary index [1,11,12]:

$$Ha = Ha(G) = \sum_{u < v} \frac{1}{d(u, v)^2} \quad (3)$$

and the reciprocal Wiener index [13–15]:

$$RW = RW(G) = \sum_{u < v} \frac{1}{d(u, v)} . \quad (4)$$

It is worth noting that all the above structure–descriptors are either special cases of, or are simply related to the graph invariant W_λ , defined as [16–18]

$$W_\lambda = W_\lambda(G) = \sum_{k \geq 1} d(G, k) k^\lambda \quad (5)$$

where $d(G, k)$ is the number of pairs of vertices of the graph G whose distance is k , and where λ is some real (or complex) number. Evidently,

$$\begin{aligned} W &= W_1 \\ WW &= \frac{1}{2} W_2 + \frac{1}{2} W_1 \\ Ha &= W_{-2} \\ RW &= W_{-1} . \end{aligned}$$

Another related quantity is the Hosoya polynomial. It was first put forward by Hosoya [19] and eventually attracted due attention by mathematicians and mathematical chemists [20–32]. Hosoya called it “the Wiener polynomial”, whereas the present name appeared for the first time in the paper [24] and was soon accepted by the majority of scholars involved in its study. With an almost 10-years delay, Sagan et al. [23] seem to have independently arrived at the very same idea as Hosoya [19].

The Hosoya polynomial is defined as

$$H(\lambda) = H(G, \lambda) = \sum_{k \geq 1} d(G, k) \lambda^k \quad (6)$$

where the notation is same as in Eq. (5). Comparing (5) and (6) we see that both W_λ and $H(\lambda)$ are determined by the numbers $d(G, k)$, $k = 1, 2, \dots$. Indeed, from knowing $H(G, \lambda)$ one can deduce $W_\lambda(G)$ and vice versa. Thus, from the Hosoya polynomial it is possible to calculate a large variety of distance-based molecular structure-descriptors, e. g. those defined via Eqs. (1)–(4).

The connection between the Hosoya polynomial and the Wiener index is elementary [19,29]:

$$W(G) = H'(G, 1)$$

where $H'(G, \lambda)$ is the first derivative of $H(G, \lambda)$. The hyper-Wiener index can be computed from the first and second derivatives as [32]

$$WW(G) = H'(G, 1) + \frac{1}{2} H''(G, 1) .$$

INTRODUCTION: THORN GRAPHS

The concept of “thorn graphs” was introduced by one of the present authors [33,34]. The thorn graph G^* is obtained from a parent n -vertex graph G by attaching $p_i \geq 0$ new pendent vertices (i. e., vertices of degree one) to the i -th vertex of G , for $i = 1, 2, \dots, n$. In [33,34] expressions for the Wiener index of various thorn graphs, including thorn trees, were obtained. Recently Bonchev and Klein [35] reported additional formulas for the Wiener index of thorn trees, thorn rods, thorn rings, and thorn stars. In this paper we obtain analogous results for the respective Hosoya polynomials.

Following the terminology proposed by Bonchev and Klein [35], if the parent graph is a tree, then we speak of “thorn trees”. In this paper we consider the case when the parent tree is a path. Then the respective thorn tree is the familiar “caterpillar” [36,37]. Under “thorn rod” is understood a caterpillar obtained so that new vertices are attached only to the two terminal vertices of the underlying path.

Another thorn tree is the “thorn star”, obtained by attaching pendent vertices to the vertices of a star, except to its central vertex.

If the parent graph is a cycle, then we speak of “thorn cycles”.

Further details as well as examples can be found elsewhere [35].

THE MAIN RESULTS

By $T(b_1, b_2, \dots, b_\ell)$ we denote a caterpillar obtained from a path on $\ell + 2$ vertices labelled consecutively as $u_1, u_2, \dots, u_{\ell-1}, u_\ell, u_{\ell+1}, u_{\ell+2}$, by attaching b_i pendent vertices to the vertex u_{i+1} , $i = 1, 2, \dots, \ell$.

Theorem 1. For a thorn tree $T = T(b_1, b_2, \dots, b_\ell)$, the Hosoya polynomial is of the form

$$H(T, \lambda) = a_1 \lambda + a_2 \lambda^2 + \dots + a_{\ell+1} \lambda^{\ell+1}$$

where

$$\begin{aligned} a_1 &= \sum_{i=1}^{\ell} b_i + (\ell + 1) \\ a_2 &= \sum_{i=1}^{\ell} \binom{b_i}{2} + 2 \sum_{i=1}^{\ell} b_i + \ell \\ a_3 &= \sum_{i=1}^{\ell-1} b_i b_{i+1} + \sum_{i=1}^{\ell-1} b_i + \sum_{i=2}^{\ell} b_i + (\ell - 1) \\ a_4 &= \sum_{i=1}^{\ell-2} b_i b_{i+2} + \sum_{i=1}^{\ell-2} b_i + \sum_{i=3}^{\ell} b_i + (\ell - 2) \\ &\vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \\ a_k &= \sum_{i=1}^{\ell-k+2} b_i b_{i+k-2} + \sum_{i=1}^{\ell-k+2} b_i + \sum_{i=k-1}^{\ell} b_i + (\ell - k + 2) \\ &\vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \\ a_{\ell-1} &= \sum_{i=1}^3 b_i b_{i+\ell-3} + \sum_{i=1}^3 b_i + \sum_{i=\ell-2}^{\ell} b_i + 3 \\ a_\ell &= \sum_{i=1}^2 b_i b_{i+\ell-2} + \sum_{i=1}^2 b_i + \sum_{i=\ell-1}^{\ell} b_i + 2 \\ a_{\ell+1} &= b_1 b_{\ell-1} + b_1 + b_\ell + 1 . \end{aligned}$$

Proof. Let $A = \{u_1, u_2, \dots, u_{\ell+1}, u_{\ell+2}\}$, $B_i = \{v_{i1}, v_{i2}, \dots, v_{ib_{i-1}}\}$ for $i = 2, 3, \dots, \ell + 1$, and

$$B = \bigcup_{i=2}^{\ell+1} B_i .$$

In order to demonstrate the validity of the theorem, we adopt the following notation:

$d_A(G, k)$ = number of pairs of vertices in the set A , at a distance k ,

$d_B(G, k)$ = number of pairs of vertices in the set B , at a distance k , and

$d_{AB}(G, k)$ = number of pairs of vertices, of which one is in the set A and the other in the set B .

One can easily observe that

$$a_k = d_A(G, k) + d_B(G, k) + d_{AB}(G, k) .$$

Computing these three terms in the above expression, we get the expressions for the coefficient a_i 's as in the statement of the theorem.

Corollary 1.1. By taking $\ell = b$ and $b_i = a - 2$ for $i = 1, 2, \dots, \ell$, we get the thorn tree $T(a, b)$ as defined in [35]. For it,

$$H(T(a, b), \lambda) = (ab - b + 1) \lambda + \frac{1}{2} ab(a - 1) \lambda^2 + \sum_{k=3}^{b+1} (b - k + 2)(a - 1)^2 \lambda^k .$$

The thorn rod is, by definition, a caterpillar with code $(b_1, 0, 0, \dots, 0, b_\ell)$. If this sequence is of length $p + 1$, and if $b_1 = b_\ell = t - 2$, then we get the rod $P_{p,t}$ from the paper [35]. For it we have:

Corollary 1.2. The Hosoya polynomial of $P_{p,t}$ is

$$\begin{aligned} H(P_{p,t}, \lambda) &= (2t + p - 3) \lambda + (t^3 - 3t + 2p) \lambda^2 + (2t + p - 5) \lambda^3 \\ &+ (2t + p - 6) \lambda^4 + \dots + (2t + p - k + 2) \lambda^k + \dots \\ &+ (2t - 1) \lambda^{p-1} + (2t - 2) \lambda^p + (2t - 3) \lambda^{p+1} . \end{aligned}$$

The thorn star $K_{1,n}^*$ with code (b_1, b_2, \dots, b_n) is the graph obtained by adding b_i pendent vertices to the i -th pendent vertex of the star $K_{1,n}$. Then by a similar counting method as used in the proof of the previous theorem we obtain:

Theorem 2. The Hosoya polynomial of the thorn star $K_{1,n}^*$ with code (b_1, b_2, \dots, b_n) is

$$H(K_{1,n}^*, \lambda) = a_1 \lambda + a_2 \lambda^2 + a_3 \lambda^3 + a_4 \lambda^4$$

where

$$\begin{aligned} a_1 &= \sum_{i=1}^n b_i + n \\ a_2 &= \sum_{i=1}^n \binom{b_{i+1}}{2} + \binom{n}{2} \\ a_3 &= (n-1) \sum_{i=1}^n b_i \\ a_4 &= b_1 \sum_{i=2}^n b_i + b_2 \sum_{i=3}^n b_i + b_{n-1} b_n . \end{aligned}$$

In [35] the thorn star $S_{k,t}$ was considered, the code of which is the k -tuple $(t-1, t-1, \dots, t-1)$.

Corollary 2.1.

$$H(S_{k,t}, \lambda) = k t \lambda + \frac{k}{2} [t(t-1) + (k-1)] \lambda^2 + k(k-1)(t-1) \lambda^3 + \frac{1}{2} k(k-1)(t-1)^2 \lambda^4 .$$

If C_n is the n -vertex cycle, then the thorn ring C_n^* with code (b_1, b_2, \dots, b_n) is obtained by adding b_i pendent vertices to the i -th vertex of C_n , $i = 1, 2, \dots, n$.

Theorem 3. For a thorn ring C_n^* with code (b_1, b_2, \dots, b_n) , the Hosoya polynomial is of the form

$$H(\lambda) = a_1 \lambda + a_2 \lambda^2 + a_3 \lambda^3 + \dots + a_{\lfloor n/2 \rfloor + 2} \lambda^{\lfloor n/2 \rfloor + 2} \quad (7)$$

where

$$a_1 = \sum_{i=1}^n b_i + n \quad ; \quad a_2 = \sum_{i=1}^n \binom{b_{i+2}}{2}$$

for $3 \leq k \leq \lfloor n/2 \rfloor$,

$$a_k = \sum_{i=1}^n b_i b_{i+k-2} + 2 \sum_{i=1}^n b_i + d(C_n, k)$$

and

$$a_{\lfloor n/2 \rfloor + 1} = \sum_{i=1}^n b_i b_{i+k-2} + \sum_{i=1}^n b_i .$$

In addition, if n is even, then

$$a_{n/2+2} = \sum_{i=1}^{n/2} b_i b_{i+n/2} . \quad (8)$$

In the above expressions the subscripts $i + k - 2$ are assumed to take the values modulo n .

Proof. The method of the proof is analogous to that of Theorem 1: we separately consider distances between pairs of vertices of C_n , between pairs of pendent vertices of C_n^* , and between pairs of vertices of which one belongs to C_n and the other is pendent.

For the case when n is even, for $k = n/2$, $k = n/2 + 1$, and $k = n/2 + 2$, we have

$$a_{n/2} = \sum_{i=1}^n b_i b_{i+n/2-2} + 2 \sum_{i=1}^n b_i + \frac{n}{2}$$

$$a_{n/2+1} = \sum_{i=1}^n b_i b_{i+n/2-1} + \sum_{i=1}^n b_i$$

and formula (8), because of the symmetric nature of even cycles.

For the special case of thorn cycles $C_{n,t}^*$, considered in [35], for which the code is $(t-2, t-2, \dots, t-2)$, we have:

Corollary 3.1. For the thorn cycle $C_{n,t}^*$, obtained from C_n by attaching to each of its vertices $t-2$ pendent vertices, the coefficients of the Hosoya polynomial, as specified in Eq. (7), are

$$a_1 = n(t-2) + n \quad ; \quad a_2 = n \binom{t}{2}$$

$$a_k = n(t-1)^2$$

for $k \geq 3$ and odd n , whereas for n being even,

$$a_k = n(t-1)^2 \quad \text{for } 3 \leq k \leq \frac{n}{2}$$

$$a_{n/2+1} = n t(t-2) \quad ; \quad a_{n/2+2} = n(t-2)^2 .$$

DISCUSSION

By means of the above results we extended the results for the Wiener indices, obtained by Bonchev and Klein, to the Hosoya polynomials. The Bonchev–Klein

results are now obtained from ours, as simple special cases. Our results, in turn, make it possible to compute not only the Wiener indices, but also the hyper-Wiener, Harary, and reciprocal Wiener indices of the thorn graphs considered, as well as their general W_λ -index.

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