The Hosoya polynomial of distance-regular graphs

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Abstract

In this note we obtain an explicit formula for the Hosoya polynomial of any distance-regular graph in terms of its intersection array. As a consequence, we obtain a very simple formula for the Hosoya polynomial of any strongly regular graph.

1 Introduction

Throughout this paper $G = (V, E)$ denotes a connected, simple and finite graph with vertex set $V = V(G)$ and edge set $E = E(G)$.

The distance $d(u, v)$ between two vertices $u$ and $v$ is the minimum of the lengths of paths between $u$ and $v$. The diameter $D$ of a graph $G$ is defined as

$$D := \max_{u, v \in V(G)} \{d(u, v)\}.$$
The Wiener index $W(G)$ of a graph $G$ with vertex set $\{v_1, v_2, \ldots, v_n\}$, defined as the sum of distances between all pairs of vertices of $G$,

$$W(G) := \frac{1}{2} \sum_{i=1,j=1}^{n} d(v_i, v_j),$$

is the first mathematical invariant reflecting the topological structure of a molecular graph.

This topological index has been extensively studied; for instance, a comprehensive survey on the direct calculation, applications, and the relation of the Wiener index of trees with other parameters of graphs can be found in [5]. Moreover, a list of 120 references of the main works on the Wiener index of graphs can be found in the referred survey.

The Hosoya polynomial of a graph was introduced in the Hosoya’s seminal paper [7] in 1988 and received a lot of attention afterwards. The polynomial was later independently introduced and considered by Sagan, Yeh, and Zhang [9] under the name Wiener polynomial of a graph. Both names are still used for the polynomial but the term Hosoya polynomial is nowadays used by the majority of researchers. The main advantage of the Hosoya polynomial is that it contains a wealth of information about distance based graph invariants. For instance, knowing the Hosoya polynomial of a graph, it is straightforward to determine the Wiener index of a graph as the first derivative of the polynomial at the point $t = 1$. Cash [3] noticed that the hyper-Wiener index can be obtained from the Hosoya polynomial in a similar simple manner. Also, Estrada et al. [6] studied several chemical applications of the Hosoya polynomial.

Let $G$ be a connected graph of diameter $D$ and let $d(G, k), k \geq 0$, be the number of vertex pairs at distance $k$. The Hosoya polynomial of $G$ is defined as

$$H(G, t) := \sum_{k=1}^{D} d(G, k) \cdot t^k.$$ 

As we pointed out above, the Wiener index of a graph $G$ is determined as the first derivative of the polynomial $H(G, t)$ at $t = 1$, i.e.,

$$W(G) = \sum_{k=1}^{D} k \cdot d(G, k).$$
The Hosoya polynomial has been obtained for trees, composite graphs, benzenoid graphs, tori, zig-zag open-ended nanotubes, certain graph decorations, armchair open-ended nanotubes, zigzag polyhex nanotori, $TUC_4C_8(S)$ nanotubes, pentachains, polyphenyl chains, the circumcoronene series, Fibonacci and Lucas cubes, Hanoi graphs, etc. See the references in [4].

In this note we obtain an explicit formula for the Hosoya polynomial of any distance-regular graph. As a consequence, we obtain a very simple formula for the Hosoya polynomial of any strongly regular graph.

2 The Hosoya polynomial of distance-regular graphs

A distance-regular graph is a regular connected graph with diameter $D$, for which the following holds. There are natural numbers $b_0, b_1, ..., b_{D-1}, c_1 = 1, c_2, ..., c_D$ such that for each pair $(u, v)$ of vertices satisfying $d(u, v) = j$ we have

1. the number of vertices in $G_{j-1}(v)$ adjacent to $u$ is $c_j$ ($1 \leq j \leq D$),
2. the number of vertices in $G_{j+1}(v)$ adjacent to $u$ is $b_j$ ($0 \leq j \leq D - 1$),

where $G_i(v) = \{ u \in V(G) : d(u, v) = i \}$.

The array $\{b_0, b_1, ..., b_{D-1}; c_1 = 1, c_2, ..., c_D\}$ is the intersection array of $G$.

Classes of distance-regular graphs include complete graphs, cycle graphs, Hadamard graphs, hypercube graphs, Kneser graphs $K(n, 2)$, odd graphs and Platonic graphs [1, 2].

Theorem 1. Let $G$ be a distance-regular graph whose intersection array is

$$\{b_0, b_1, ..., b_{D-1}; c_1 = 1, c_2, ..., c_D\}.$$ 

Then we have

$$H(G, t) = \frac{nb_0}{2} \left( t + \sum_{i=2}^{D} \frac{\prod_{j=1}^{i-1} b_j}{\prod_{j=2}^{i} c_j} \cdot t^i \right).$$
Proof. For any vertex \( v \in V(G) \), each vertex of \( G_{i-1}(v) \) is joined to \( b_{i-1} \) vertices in \( G_i(v) \) and each vertex of \( G_i(v) \) is joined to \( c_i \) vertices in \( G_{i-1}(v) \). Thus

\[
|G_{i-1}(v)| b_{i-1} = |G_i(v)| c_i. \tag{1}
\]

Hence, it follows from (1) that the number of vertices at distance \( i \) of a vertex \( v \), namely \( |G_i(v)| \), is obtained directly from the intersection array

\[
|G_i(v)| = \prod_{j=0}^{i-1} b_j \prod_{j=2}^{i} c_j \quad (2 \leq i \leq D) \quad \text{and} \quad |G_1(v)| = b_0. \tag{2}
\]

Now, since, \( d(G, i) = \frac{1}{2} \sum_{v \in V(G)} |G_1(v)| \) and the value \( |G_1(v)| \) does not depend on \( v \), we obtain the following:

\[
d(G, i) = \frac{n \prod_{j=0}^{i-1} b_j}{2 \prod_{j=2}^{i} c_j} \quad (2 \leq i \leq D) \quad \text{and} \quad |G_1(v)| = \frac{nb_0}{2}. \tag{3}
\]

Therefore, the result is a direct consequence of the definition of the Hosoya polynomial. \( \square \)

As an example, the hypercubes \( Q_k, \ k \geq 2 \), are distance-regular graphs whose intersection array is \( \{k, k-1, \ldots, 1; 1, 2, \ldots, k\} \). Thus, from Theorem 1 we obtain that the Hosoya polynomial of the hypercube \( Q_k \) is

\[
H(Q_k, t) = 2^{k-1} \sum_{i=1}^{k} \binom{k}{i} t^i = 2^{k-1} ((t + 1)^k - 1).
\]

As a direct consequence of Theorem 1 we deduce the formula on the Wiener index of a distance-regular graph, which was previously obtained in \( \square \) for the general case of hypergraphs.

**Corollary 2.** \( \square \) Let \( G \) be a distance-regular graph whose intersection array is

\( \{b_0, b_1, \ldots, b_{D-1}; c_1 = 1, c_2, \ldots, c_D\} \).

Then we have

\[
W(G) = \frac{nb_0}{2} \left( 1 + \sum_{i=2}^{D} \frac{\prod_{j=1}^{i-1} b_j}{\prod_{j=2}^{i} c_j} \right).
\]
A graph is said to be \(k\)-regular if all vertices have the same degree \(k\). A \(k\)-regular graph \(G\) of order \(n\) is said to be strongly regular, with parameters \((n, k, \lambda, \mu)\), if the following conditions hold. Each pair of adjacent vertices has the same number \(\lambda \geq 0\) of common neighbours, and each pair of non-adjacent vertices has the same number \(\mu \geq 1\) of common neighbours (see, for instance, [II]). A distance-regular graph of diameter \(D = 2\) is simply a strongly regular graph. In terms of the intersection array \(\{b_0, b_1; 1, c_2\}\) we have that \(\lambda = k - 1 - b_1\) and \(\mu = c_2\), i.e., the intersection array of any strongly regular graph with parameters \((n, k, \lambda, \mu)\) is \(\{k, k - \lambda - 1; 1, \mu\}\). Thus, as a consequence of Theorem III we deduce the following result.

**Corollary 3.** Let \(G\) be a strongly regular graph with parameters \((n, k, \lambda, \mu)\). Then we have

\[
H(G, t) = \frac{nk}{2} \left( t + \frac{k - \lambda - 1}{\mu} \cdot t^2 \right).
\]

It is well-known that the parameters \((n, k, \lambda, \mu)\) of any strongly regular graph are not independent and must obey the following relation:

\[(v - k - 1)\mu = k(k - \lambda - 1)\]

As a result, we can express the Hosoya polynomial of any strongly regular graph in the following manner

\[
H(G, t) = \frac{n}{2} (kt + (n - k - 1)t^2);
\]

this is not surprising because for every vertex \(x\) there are \(k\) vertices at distance 1 from \(x\) and \(n - k - 1\) at distance 2 (since a strongly regular graph has diameter \(D = 2\)).

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