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On the Degeneracy of the Orbit Polynomial and Related Graph Polynomials

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Abstract: The orbit polynomial is a new graph counting polynomial which is defined as $O_G(x) = \sum_{i=1}^{r} x^{|O_i|}$, where $O_1, \ldots, O_r$ are all vertex orbits of the graph G. In this article, we investigate the structural properties of the automorphism group of a graph by using several novel counting polynomials. Besides, we explore the orbit polynomial of a graph operation. Indeed, we compare the degeneracy of the orbit polynomial with a new graph polynomial based on both eigenvalues of a graph and the size of orbits.

Keywords: automorphism group; orbit; group action; polynomial roots; orbit-stabilizer theorem

1. Introduction

In quantum chemistry, the early Hückel theory computes the levels of π-electron energy of the molecular orbitals in conjugated hydrocarbons, as roots of the characteristic/spectral polynomial which are called the eigenvalues of a molecular graph, see [1]. This concept was generalized by Hosoya [2] and the others [3–5] by changing the adjacency matrix with other matrices based on graph invariants. In the mathematical chemistry literature, the counting polynomials have first been introduced by Hosoya, see [6]. Other counting polynomials have later been proposed: Matching polynomial [7,8], independence [9,10], king [11,12], color [12], star or clique polynomials [13,14], etc. An overview of graph polynomials is provided in reference [15].

In the current work, we introduce a novel graph polynomial based on orbit-partitions of regarding graph, see [16,17]. It is derived from the concept of orbit polynomial. The typical terms of the orbit polynomial is of the form $c_n x^n$, where c_n is the number of orbits of the automorphism group of size n. It should be noted that the characteristic polynomials do not characterize graphs due to several isospectral graphs, see [18].

We proceed as follows. In Section 2, the definitions used in the present work are introduced and known results needed are given. Section 3, contains the main results of this paper based on the orbit structure of a graph. Finally, in Section 4, by using the concept of graph spectra, we define a new version of orbit polynomial whose unique positive root is a measure that discriminate all graphs of order six, uniquely.

2. Preliminaries

In this research, $V(G)$ and $E(G)$ indicates the vertex and edge sets of the graph G, respectively. We assume that all graphs are simple, connected and finite.

In this paper, the automorphism group of a graph as well as the vertex-orbits are needed to infer the orbit polynomial. The automorphism group is a collection of all permutations on the set of vertices that preserves the adjacency between vertices of a graph, namely $e = xy$ is an edge of graph G if and only if $\pi(e) = \pi(x)\pi(y)$ is an edge. We denote the automorphism group of a graph G by Aut(G).

For the vertex u, an orbit containing u is the collection of all $\alpha(v)$'s in which α is an automorphism element of G. The graph G is said to be vertex-transitive, if it has exactly one orbit. This means that in a vertex-transitive all vertices can be mapped to each other, namely for two elements a and b, there is at least an automorphism β that $\beta(a) = b$. An edge-transitive graph can be defined similarly.

Let Γ be a group acting on the set X. The stabilizer of element $x \in X$ is defined as $\Gamma_x = \{g \in \Gamma : g.x = x\}$. The orbit-stabilizer theorem implies that $|x^\Gamma| \times |\Gamma_x| = |\Gamma|$, see [19].

3. The Orbit and the Modified Orbit Polynomials

The orbit polynomial was defined by Dehmer et al. in [16] as

$$O_G(x) = \sum_{i=1}^{t} x^{|O_i|},$$

where $O_1, \ldots O_t$ are all vertex-orbits of G. Moreover, the the modified version of orbit polynomial, $O^\star_G$ is defined as

$$O^\star_G(x) = 1 - \sum_{i=1}^{t} x^{|O_i|}.$$

Many structural properties of a graph can be derived from the orbit polynomial. Let G be a graph of order n. From the definition, it is clear that if $Aut(G) \cong id$, then $O_G(x) = nx$ and thus $O^\star_G(x) = 1 - nx$. Moreover, a graph is vertex-transitive if and only if $O_G(x) = x^n$ and consequently $O^\star_G(x) = 1 - x^n$.

Example 1. *The cycle graph C_n is vertex-transitive and by the above discussion $O_{C_n}(x) = x^n$ and $O^\star_{C_n}(x) = 1 - x^n$.*

Example 2. *For the path graph P_n we obtain*

$$O_{P_n}(x) = \begin{cases} \frac{n}{2}x^2, & 2 \mid n \\ x + \frac{n-1}{2}x^2, & 2 \not| n \end{cases},$$

and

$$O^\star_{P_n}(x) = \begin{cases} 1 - \frac{n}{2}x^2, & 2 \mid n \\ 1 - x - \frac{n-1}{2}x^2, & 2 \not| n \end{cases}.$$

From the orbit polynomial P_n, one can easily see that if n is even then P_n has a pendant edge and if n is odd then P_n has a central vertex, since each tree has a central vertex or a central edge, see [20]. We also explore that in the case that n is even (n is odd), then P_n has $\frac{n}{2}$ ($\frac{n-1}{2}$) orbits of length two.

3.1. Orbit Polynomial of Line Graphs

An edge-automorphism of graph G is a bijection α on $E(G)$ such that two edges e, f are adjacent if and only if $\alpha(e)$ and $\alpha(f)$ are adjacent in G. The set of all edge-automorphisms of graph G is also a group under the composition of functions and we denote it by $Aut_1(G)$.

Any automorphism α of G induces a bijection $\bar{\alpha}$ on $E(G)$, defined by $\bar{\alpha}(uv) = \alpha(u)\alpha(v)$. It is clear that $\bar{\alpha}$ is an edge-automorphism. The set

$$Aut^{\star}(G) = \{\bar{\alpha} : \alpha \in Aut(G)\}$$

is a subgroup of $Aut(G)$ induced by edge-automorphisms of G.

Theorem 3 ([20])**.** *Assume that G is a graph of order $n \geq 3$. Then $Aut(G) \cong Aut^{\star}(G)$.*

For a graph G, its line graph $\mathcal{L}(G)$ is a new graph with the vertex set is $E(G)$ and two vertices are adjacent in $\mathcal{L}(G)$ if and only if the corresponding edges are adjacent in G. An automorphism of $\mathcal{L}(G)$ is an edge-automorphism of G. Suppose $\mathcal{W} = \{W_1, W_2, W_3\}$ are the set of graphs as depicted in Figure 1. Then we have the following theorem.

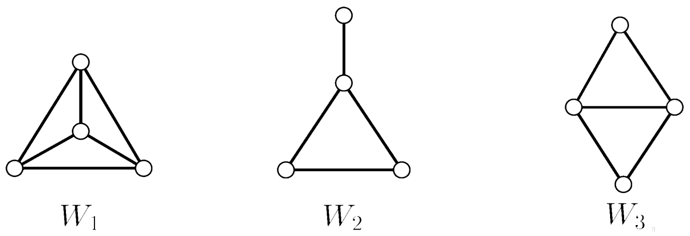

Figure 1. Three graphs W_1, W_2 and W_3 of order 4.

Theorem 4 ([1])**.** *For a connected graph G, where $G \notin \mathcal{W}$, we have*

$$Aut(G) \cong Aut(\mathcal{L}(G)).$$

Consider two graphs G_1 and $\mathcal{L}(G_1)$ in Figure 2. Both of them have the same orbit polynomial $O_{G_1}(x) = O_{\mathcal{L}(G_1)}(x) = 2x^2 + x$ while for two graphs G_2 and $\mathcal{L}(G_2)$ in Figure 3, we have $O_{G_2}(x) = x^2 + x^4$ and $O_{\mathcal{L}(G_2)}(x) = x^3 + x$. Finally, consider the graph G_3 and its line graph as depicted in Figure 4. The automorphism group of both of them is isomorphic with symmetric group $\mathbb{S}_3$ but $O_{G_3}(x) = x + x^3$ and $O_{\mathcal{L}(G_3)}(x) = x^3$.

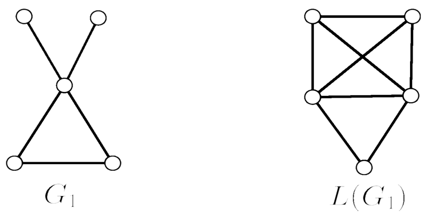

Figure 2. A graph with its line graph, both of order 5.

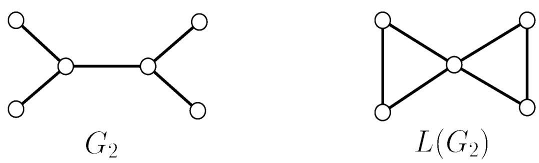

Figure 3. A graph of order 6 whose line graph is of order 5.

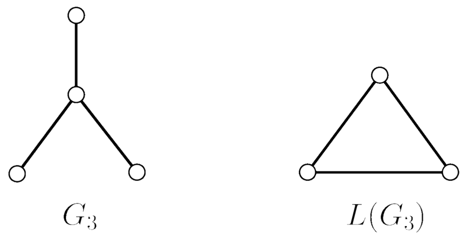

Figure 4. A graph and its line graph which have the same automorphism group.

The distance between two vertices x and y a graph G is the length of the shortest path between them and we denote it by $d(x, y)$. For the vertex u of graph G, suppose $\Gamma_i(u)$ is the number of vertices at distance i from u. If for two vertices u and v, we have $\Gamma_i(u) = \Gamma_i(v)$ $(1 \leq i \leq d(G))$ then they are Hosoya-equivalent or H-equivalent, see [21–30].

The set of H-equivalent vertices is called an H-partition of G. Moreover, the Hosoya polynomial is defined as $P_G(x) = \sum_{i=1}^{l} x^{h_i}$, where $H_1, \ldots, H_l$ are all H-partitions of G and $h_i = |H_i|$. The modified Hosoya polynomial is also $P^\star_G(x) = 1 - P_G(x)$.

Theorem 5. *Suppose $O_1, \ldots, O_r$ are all orbits of graph G. If for any pair of vertices $v_i \in O_i$ and $v_j \in O_j$, we have $\deg(v_i) \neq \deg(v_j)$ $(1 \leq i, j \leq r)$, then O_i's are all H-partitions of G.*

Proof. It is clear that two vertices in the same orbit have the same degree. Moreover, two vertices u and v in a same H-partition have the same degree, since $dds(u) = dds(v)$ yields that $s_1(u) = s_1(v)$. Thus, if vertices of different orbits have different degrees, then they are in different H-partitions. This completes the proof. □

Corollary 6. *If the degrees of orbit vertices are distinct, then the orbit and Hosoya polynomials are the same, namely*

$$O_G(x) = P_G(x) \text{ and } O^\star_G(x) = P^\star_G(x).$$

By considering the definition of action of automorphism group of graph G on the set of edges, the edge version of orbit polynomial can be defined as follows.

Definition 7. *Let $E_1, \ldots E_h$ are all edge-orbits under the action of $Aut(G)$ on the set of edges. Then*

$$\bar{O}_G(x) = \sum_{i=1}^{h} x^{|E_i|},$$

$$\bar{O}^\star_G(x) = 1 - \sum_{i=1}^{h} x^{|E_i|}.$$

For example, the star graph S_n is edge-transitive; hence $\bar{O}_{S_n} = x^{|E|} = x^{n-1}$ and $\bar{O}^\star_{S_n} = 1 - x^{n-1}$. On the other hand, if T is a tree on n vertices with $\bar{O}_T(x) = x^{n-1}$, then T is edge-transitive and so T is a bi-regular graph, which means that all vertices of T are of degrees r and s for some $r, s \in \mathbb{N}$. If T is regular, then $T \cong K_2$ which confirms our claim. If T is a bi-regular tree, then $T \cong S_n$, since the pendant vertices compose an orbit and the central vertex is a singleton orbit. Notice that if $n \geq 3$, then an edge-transitive tree has not a central edge. Hence, we proved the following theorem.

Theorem 8. *The edge-orbit polynomial $\bar{O}_T(x) = x^{n-1}$ if and only if $T \cong S_n$.*

In continuing this section, we prove that the cycle graph C_n can be characterized by its edge-orbit polynomial.

Theorem 9. *Let G be a graph without a pendant edge. Then $O_G(x) = \bar{O}_G(x)$ if and only if $G \cong C_n$.*

Proof. If $G \cong C_n$, then we are done. Conversely, by $O_G(x) = \bar{O}_G(x)$, one can immediately conclude that the number of edges and the number of vertices of graph G are the same and thus G is a unicycle graph. If G has a vertex of degree greater than two, then G has at least two cycles, a contradiction. Hence, G is a connected regular graph of degree 2 and the assertion follows. □

Suppose G is a graph with k orbits of equal sizes. Then $O_G(x) = kx^{\frac{n}{k}}$ and thus zero is the only root of O_G. On the other hand, if $x = 0$ is the only root of O_G, then $O_G(x) = kx^t$, for some $k, t \in \mathbb{N}$. However, the set of orbits of a graph is a partition of the vertex set and thus $kt = n$, which means that $t = \frac{n}{k}$. In particular, if $k = 1$ then G is vertex-transitive and if $k = n$ then G is asymmetric graph. Hence, we proved the following theorem.

Theorem 10. *The integer $x = 1$ is a root of $O^\star_G(x)$ if and only if G is vertex-transitive.*

Proof. If G is vertex-transitive, then $O^\star_G(x) = 1 - x^n$ and clearly $x = 1$ is a zero of it. Conversely, if $x = 1$ is a zero of $O^\star_G(x) = 1 - \sum_{i=1}^r a_i x^{|O_i|}$, then $O^\star_G(1) = 1 - a_1 - \ldots - a_r = 0$. Since, $a_i \geq 1$, necessarily $r = 1$ and $a_1 = 1$ which yields that G is vertex-transitive as desired. □

3.2. Graph Classification with Respect to Orbit Polynomial

One of the classical problem in algebraic graph theory is characterizing the graphs in terms of the graph polynomials. Here, we introduce three classes of trees that can be characterized by their orbit polynomials.

Theorem 11. *If G is a graph with orbit polynomial $x + x^2 + x^3$, then G is a graph on 6 vertices. Moreover, if G has a pendant edge, then it has three pendant edges.*

Proof. Clearly, G has 6 vertices, since the set of orbits is a partition for the vertex set. If G has only one pendant edge, then its endpoints compose two different singleton orbits, a contradiction. If G has two pendant edges, then necessarily they compose an orbit of size two. These edges share a common vertex, because in other case either we have two orbits of sizes 2 and 4 or three orbits of size two or there are two orbits of size 2, all of them are contradictions. Hence, three other vertices are in the same orbit and they have the same degree. If they are of degree 2, then $G \cong (K_3 \cup \bar{K}_2) + K_1$ or $G \cong C_4 + 3e$. If $G \cong C_4 + 3e$, then $O_G(x) = 2x + 2x^2$, a contradiction. □

Example 12. *All graphs on six vertices with the orbit polynomial $O_G(x) = x + x^2 + x^3$ are as depicted in Figure 5. They have different automorphism groups while their orbit polynomials are the same.*

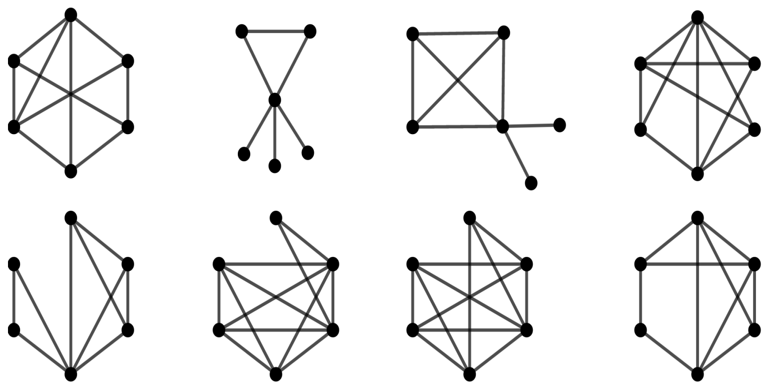

Figure 5. All graphs on six vertices with orbit polynomial $x + x^2 + x^3$.

Example 13. *Suppose $O_G(x) = ax + bx^2 + cx^3$. Then $O_G(1) = a + 2b + 3c = n$, $(1 \leq a, b, c \leq 3)$ and thus $6 \leq n \leq 18$. All graphs with this property have at least six and at most 18 vertices. The problem is solved completely for $n = 6$. If $n = 7$, then necessarily $a = 2$ and $b = c = 1$. Hence, $O_G(x) = 2x + x^2 + x^3$. This means that the related graph has two orbits of size 1, an orbit of size 2 and an orbit of size 3. There are 39 graphs of order 7 by this property. Some of them are depicted in Figure 6.*

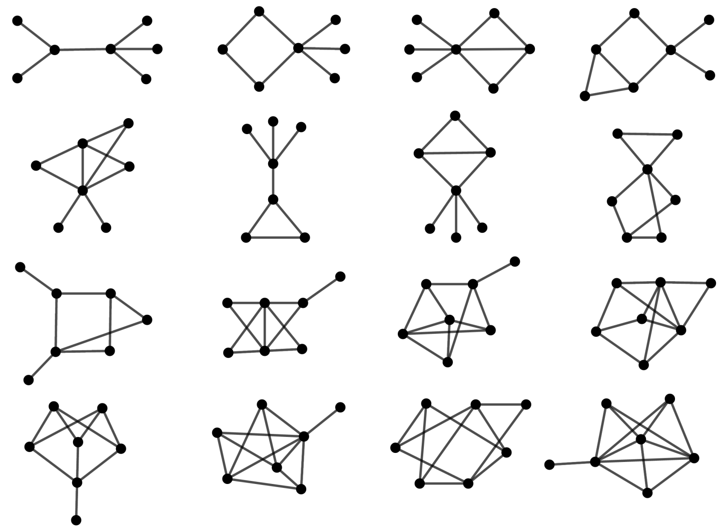

Figure 6. Examples of graphs of order 7 with orbit polynomial $2x + x^2 + x^3$.

If $n = 8$, then $O_G(x) = 3x + x^2 + x^3$ or $O_G(x) = x + 2x^2 + x^3$, see Figure 7. Since the orbit sizes are $1, 2, 3$, then by orbit-stabilizer theorem, we obtain

$$2, 3 \mid |Aut(G)| \text{ and } gcd(2, 3) = 1, \tag{1}$$

and thus $6 \mid |Aut(G)|$. On the other hand, G has no a permutation of order 6, since otherwise we have a singleton orbit. Moreover, by a similar argument, we can show that there is no permutation of order 5 or 4. This means that G is a $\{2, 3\}$ group and thus $|Aut(G)| = 2^\alpha.3^\beta$, since all orbits are of sizes $1, 2, 3$. If for example, we have only one orbit of each size 1, 2 and 3, then $|Aut(G)| = 2^\alpha.3^\beta$, where $\alpha \in \{0, 1\}$ and $\beta \in \{0, 1\}$. This means that by applying Equation (1), $|Aut(G)| = 6$ or 12 and thus $Aut(G) \cong \mathbb{Z}_6$ or $\mathbb{S}_3$ or $\mathbb{Z}_2 \times \mathbb{S}_3$. Hence, we proved the following theorem.

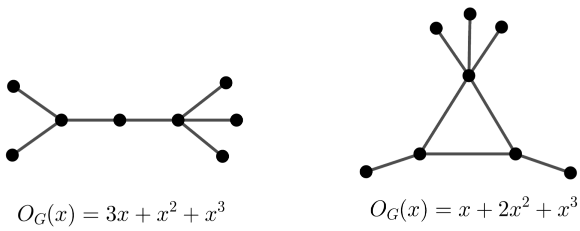

Figure 7. Two graphs of order 8 with three distinct orbit sizes.

Theorem 14. *Let G be a graph of order 6. Then $O_G(x) = x + x^2 + x^3$ if and only if $Aut(G) \cong \mathbb{Z}_6$ or $\mathbb{S}_3$ or $\mathbb{Z}_2 \times \mathbb{S}_3$.*

4. Orbit-Entropy Polynomial

The characteristic polynomial [1] of a graph G with adjacency matrix $A(G)$ is

$$\chi(G, \lambda) = \det(\lambda I - A(G)).$$

The roots of this polynomial are eigenvalues of G and form the spectrum of G as

$$spec(G) = \{[\lambda_1]^{m_1}, [\lambda_2]^{m_2}, \ldots, [\lambda_r]^{m_r}\},$$

where m_i $(1 \leq i \leq r)$ is the multiplicity of eigenvalue λ_i and $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_r$.

Here, consider all graphs of order six and their orbit polynomials as reported in Tables 1 and 2. There are 13 graphs with the same orbit polynomial $O_G = x^2 + x^4$. This means that the orbit polynomial has not a power discrimination to characterize all graphs of the same order. In [16], it is claimed that the degeneracy of roots of the modified version of orbit polynomial is less than orbit polynomial, but for the 13 mentioned graph of order 6, we obtain $O_G^{\star} = 1 - x^2 - x^4$ which implies that the modified orbit polynomial is not also a powerful discrimination to capture structural information for these graphs. Here, we introduce a new polynomial with more powerful discrimination than orbit polynomial, to capture structural information.

A number of measures using Shannon's entropy function have been introduced and investigated since the fifties, see [31–34]. The discrete form of this well-known function is defined for a probability vector $p = (p_1, p_2, \ldots, p_n)$ and has the form $I(p) = -\sum_{i=1}^{n} p_i \log(p_i)$; see [35,36].

Let $\lambda_1, \ldots, \lambda_s$ be all non-zero eigenvalues of a graph G. Then $I_\lambda(G)$ is called the eigenvalue-entropy based on λ_i's, where

$$I_\lambda(G) = -\sum_{i=1}^{s} \frac{c_i|\lambda_i|}{\sum_{j=1}^{s} c_j|\lambda_j|} \log\left(\frac{c_i|\lambda_i|}{\sum_{j=1}^{s} c_j|\lambda_j|}\right). \tag{2}$$

If $c_1 = c_2 = \ldots = c_s$, then the Equation (2) can be reformulated as follows:

$$I_\lambda(G) = -\sum_{i=1}^{s} \frac{|\lambda_i|}{\mathcal{E}(G)} \log\left(\frac{|\lambda_i|}{\mathcal{E}(G)}\right),$$

where $\mathcal{E}(G) = \sum_{j=1}^{s} |\lambda_j|$ is the adjacency energy of graph G, see [5,37].

The degeneracy problem of orbit polynomial can be overcome, by constructing the so-called super polynomial which is defined by subtracting the orbit polynomial from eigenvalue entropy:

$$\tilde{O}_G(x) = I_\lambda(G) - \sum_{i=1}^{r} x^{|O_i|} = I_\lambda(G) - O_G(x).$$

The unique positive roots (δ) of the orbit-entropy polynomials $\tilde{O}_G$ for all graphs of order six is reported in the third column of Table 1. Comparing these quantities with the orbit polynomial roots, we obtain that δ's are distinct, for all these 13 graphs.

Bear in mind that two vertex-transitive graphs of the same order have the same orbit polynomials and thus the same modified orbit polynomials. However, in general, their orbit-entropy polynomials are not equal. For example, consider two graphs $\mathcal{H}_1$ and $\mathcal{H}_2$ in Figure 8. The spectrum of these graphs are

$$spec(\mathcal{H}_1) = \{[-3]^1, [0]^4, [3]^1\},$$

and

$$spec(\mathcal{H}_2) = \{[-2]^2, [0]^2, [1]^1, [3]^1\}.$$

Then $I_\lambda(\mathcal{H}_1) = 1$ and $I_\lambda(\mathcal{H}_2) = 1.41$. Hence, $\tilde{O}_{\mathcal{H}_1} = 1 - x^6$, and $\tilde{O}_{\mathcal{H}_2} = 1.41 - x^6$ while the orbit polynomial of both of them is $O_{\mathcal{H}_i} = x^6, i = 1, 2$.

Table 1. All graphs of order six together with their unique positive roots of $O_G^\star$ and $\tilde{O}_G$.

Edges	$O_G(x)$	δ_1	δ_2
12 15 16 23 34 36 45 56	x^6	1	0.6702212
12 14 16 23 25 34 36 45 56	x^6	0.1666667	1
12 13 14 16 23 24 25 35 36 45 46 56	x^6	1	1.0699132
12 13 14 25 36 45 46 56	x^6	0.1666667	1.113457
12 13 14 15 16 23 24 25 26 34 35 36 45 46 56	x^6	1	1.1383303
12 16 23 34 45 56	x^6	1	1.164993
12 13 14 15 16 23 26 34 45 56	$x^5 + x$	0.7548777	0.4729019
12 13 14 15 16	$x^5 + x$	0.7548777	0.7548777
12 13 14 15 16 26 36 46 56	$x^4 + x^2$	0.7861514	0.8941061
12 13 14 15 26 36 46 56	$x^4 + x^2$	0.7861514	0.9495666
12 13 24 25 34 35 46 56	$x^4 + x^2$	0.7861514	0.9550358
12 13 14 15 16 23 24 25 26 34 35 46 56	$x^4 + x^2$	0.7861514	0.9586942
12 13 14 45 46	$x^4 + x^2$	0.7861514	0.986161
12 13 14 15 16 23 24 25 26 34 35 36 45 46	$x^4 + x^2$	0.7861514	0.9962842
12 13 14 15 23 24 26 34 35 46 56	$x^4 + x^2$	0.7861514	1.017727
12 13 14 23 24 35 36 45 46 56	$x^4 + x^2$	0.7861514	1.018589
12 13 23 24 34 45 46 56	$x^4 + x^2$	0.7861514	1.032434
12 13 15 24 26 34 56	$x^4 + x^2$	0.7861514	1.043184
12 13 23 24 25 34 35 45 46 56	$x^4 + x^2$	0.7861514	1.048236
12 13 14 23 24 34 35 36 45 46 56	$x^4 + x^2$	0.7861514	1.053093
12 13 23 34 45 46 56	$x^4 + x^2$	0.7861514	1.064051
12 23 24 25 26 34 35 36 45 46 56	$x^4 + 2x$	0.4746266	0.8519102
12 13 14 15 16 23 45	$x^4 + 2x$	0.4533977	0.866788
12 14 16 23 24 25 26 34 36 45 46 56	$2x^3$	0.7937005	0.9545863
12 13 14 23 25 36	$2x^3$	0.7937005	1.052146
12 16 23 24 26 34 45 46 56	$2x^3$	0.7937005	1.0553004
12 13 14 15 16 24 26 34 36 45 56	$x^3 + x^2 + x$	0.543689	0.6815621
12 14 15 16 23 25 34 36 45 56	$x^3 + x^2 + x$	0.543689	0.7255892
12 13 14 15 16 56	$x^3 + x^2 + x$	0.543689	0.7655241
12 13 14 16 23 24 26 34 45 56	$x^3 + x^2 + x$	0.543689	0.8057402
12 13 14 15 16 45 46 56	$x^3 + x^2 + x$	0.543689	0.8307845
12 13 14 23 24 25 26 34 35 36 45 46 56	$x^3 + x^2 + x$	0.543689	0.8466243
12 13 23 24 25 26 34 35 36 45 46 56	$x^3 + x^2 + x$	0.543689	0.8593803
12 13 14 23 24 34 45 46 56	$x^3 + x^2 + x$	0.543689	0.8959589
12 13 14 15 25 35 45 56	$x^3 + 3x$	0.3221854	0.5236913
12 13 14 15 36 46 56	$x^3 + 3x$	0.3221854	0.5303547
12 13 14 15 56	$x^3 + 3x$	0.3221854	0.5623349
12 13 14 23 24 25 34 35 45 56	$x^3 + 3x$	0.3221854	0.6598521
12 13 14 23 24 34 45 56	$x^3 + 3x$	0.3221854	0.7888727
12 13 14 23 24 35 36 45 46	$3x^2$	0.5773503	0.754669
12 13 14 15 35 45 56	$3x^2$	0.5773503	0.7832625
12 13 14 15 25 45 36 56	$3x^2$	0.5773503	0.7906526
12 13 14 35 45 56	$3x^2$	0.5773503	0.7941527
12 13 15 23 24 26 34 35 45 46 56	$3x^2$	0.5773503	0.8132007
12 13 14 23 24 34 35 36 45 46	$3x^2$	0.5773503	0.8189366
13 14 23 24 35 46 56	$3x^2$	0.5773503	0.8463915
12 13 24 34 35 36 45 46 56	$3x^2$	0.5773503	0.8475269
12 13 14 23 24 25 36 45 46 56	$3x^2$	0.5773503	0.8496398
12 13 14 15 16 23 24 34 35 45 46 56	$3x^2$	0.5773503	0.8570451
12 13 14 15 35 34 45 56	$3x^2$	0.5773503	0.863892
12 13 14 34 35 45 56	$3x^2$	0.5773503	0.8752257
12 16 23 26 34 35 36 45 56	$3x^2$	0.5773503	0.8791742
12 14 23 34 35 46	$3x^2$	0.5773503	0.8799624
12 23 34 45 56	$3x^2$	0.5773503	0.8943799
12 13 14 23 24 35 46 56	$3x^2$	0.5773503	0.8985653

Table 2. (Continuation of Table 1).

Edges	$O_G(x)$	δ_1	δ_2
12 13 14 15 16 34 45 56	$2x^2 + 2x$	0.3660254	0.2511261
12 13 15 16 23 34 45 56	$2x^2 + 2x$	0.3660254	0.3991883
12 14 15 16 23 34 35 36 45 56	$2x^2 + 2x$	0.3660254	0.5461031
12 13 14 35 36 45 46	$2x^2 + 2x$	0.3660254	0.5707891
12 13 14 15 46 56	$2x^2 + 2x$	0.3660254	0.5840871
12 13 14 34 35 46 56	$2x^2 + 2x$	0.3660254	0.6006301
12 13 14 15 16 23 26 34 35 45 46 56	$2x^2 + 2x$	0.3660254	0.6079497
12 13 14 15 16 23 26 34 36 46 56	$2x^2 + 2x$	0.3660254	0.6146048
12 13 23 24 25 34 35 46 56	$2x^2 + 2x$	0.3660254	0.6146802
12 13 14 15 16 34 36 45 46 56	$2x^2 + 2x$	0.3660254	0.6220295
12 13 14 15 16 23 26 34 35 45 56	$2x^2 + 2x$	0.3660254	0.6358562
12 13 14 15 24 34 45 56	$2x^2 + 2x$	0.3660254	0.6387785
12 13 14 35 36 45 46 56	$2x^2 + 2x$	0.3660254	0.6393063
12 13 14 16 23 26 34 45 46 56	$2x^2 + 2x$	0.3660254	0.6438021
12 13 14 15 16 23 45 56	$2x^2 + 2x$	0.3660254	0.6500915
12 13 14 15 23 46 56	$2x^2 + 2x$	0.3660254	0.6508345
12 13 14 15 16 23 34 35 45 56	$2x^2 + 2x$	0.3660254	0.6566663
12 13 14 15 16 45 56	$2x^2 + 2x$	0.3660254	0.6618526
12 13 14 45 46 56	$2x^2 + 2x$	0.3660254	0.6629316
12 13 14 15 16 23 34 45 56	$2x^2 + 2x$	0.3660254	0.6712485
12 13 14 15 16 45 56	$2x^2 + 2x$	0.3660254	0.6736593
12 13 14 23 24 34 35 45 56	$2x^2 + 2x$	0.3660254	0.6858483
12 13 14 35 46 56	$2x^2 + 2x$	0.3660254	0.6927251
12 13 15 16 23 26 34 45 56	$2x^2 + 2x$	0.3660254	0.6933868
12 13 14 15 23 45 46 56	$2x^2 + 2x$	0.3660254	0.7033814
12 13 14 36 45	$2x^2 + 2x$	0.3660254	0.7035179
12 15 23 34 45 46 56	$2x^2 + 2x$	0.3660254	0.7133716
12 13 14 16 23 25 34 45 56	$x^2 + 4x$	0.236068	0.409835
12 13 14 15 34 36 45 56	$x^2 + 4x$	0.236068	0.4131627
12 13 14 15 26 34 46 56	$x^2 + 4x$	0.236068	0.4183624
12 13 14 15 45 56	$x^2 + 4x$	0.236068	0.4276625
12 13 14 25 35 46	$x^2 + 4x$	0.236068	0.4343068
12 13 14 45 56	$x^2 + 4x$	0.236068	0.4411921
12 13 14 15 16 23 25 34 45 56	$x^2 + 4x$	0.236068	0.4527634
12 13 14 15 23 25 34 45 56	$x^2 + 4x$	0.236068	0.4601455
12 13 14 15 16 34 25 45 56	$x^2 + 4x$	0.236068	0.4609852
12 13 23 24 25 34 35 45 56	$x^2 + 4x$	0.236068	0.4722518
12 13 14 15 23 24 56	$x^2 + 4x$	0.236068	0.4798687
12 13 14 15 23 24 26 34 45 56	$x^2 + 4x$	0.236068	0.4853394
12 13 14 15 16 34 36 45 46	$x^2 + 4x$	0.236068	0.4879452
12 13 23 24 34 45 56	$x^2 + 4x$	0.236068	0.4913081
12 13 14 15 36 45 46 56	$x^2 + 4x$	0.236068	0.4950764
12 13 14 15 16 23 24 34 35 45 56	$x^2 + 4x$	0.236068	0.4981524
12 13 16 23 26 34 35 45 56	$x^2 + 4x$	0.236068	0.4990413
12 13 14 24 34 35 36 45 46 56	$x^2 + 4x$	0.236068	0.513049
12 13 14 15 23 45 46	$x^2 + 4x$	0.236068	0.5143182
12 13 14 15 34 56	$x^2 + 4x$	0.236068	0.5174416
12 13 14 23 45 56	$x^2 + 4x$	0.236068	0.5219741
12 13 14 15 23 34 45 56	$6x$	0.1666667	0.3597291
12 13 14 16 23 34 35 45 56	$6x$	0.1666667	0.36443
12 13 14 15 23 34 45 56	$6x$	0.1666667	0.3744274
12 13 14 15 23 34 46 56	$6x$	0.1666667	0.3752572
12 13 14 15 45 36 56	$6x$	0.1666667	0.3787899
12 13 14 15 35 36 45	$6x$	0.1666667	0.3788464
12 13 14 35 45 46 56	$6x$	0.1666667	0.3808788
12 13 14 34 45 56	$6x$	0.1666667	0.3903846

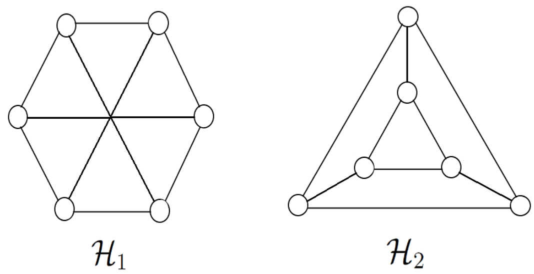

Figure 8. Two vertex-transitive graphs of order 6 with distinct orbit-entropy polynomials.

5. Summary and Conclusions

The Hosoya partition and the orbit polynomials of several kinds of graphs were investigated. Moreover, a relation between the orbit and Hosoya partition polynomials was explored. We also defined a new polynomial based on both orbit sizes and eigenvalues of a graph, and it was shown that the degeneracy of new polynomial relative to the orbit polynomial is quite low. Applying the theory of groups, especially the automorphism group approach used in this paper, enables one to analyze networks and we capture information about the number of interconnections of components. Finally, a characterization for all graphs with orbit polynomial $O_G(x) = x + x^2 + x^3$ is given.

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References

1. Cvetković, D.; Doob, M.; Sachs, H. *Spectra of Graphs Theory and Applications*; Academic Press: Heidelberg, Germany, 1995.
2. Hosoya, H. On some counting polynomials in chemistry. Applications of graphs in chemistry and physics. *Discret. Appl. Math.* **1988**, *19*, 239–257. [CrossRef]
3. Gutman, I.; Harary, F. Generalizations of the matching polynomial. *Util. Math.* **1983**, *24*, 97–106.
4. Gutman, I.; Bonchev, D.; Rouvray, D.H. *Polynomials in Graph Theory. Chemical Graph Theory, Introduction and Fundamentals*; Abacus Press: New York, NY, USA, 1991; pp. 133–176.
5. Gutman, I.; Furtula, B.; Katanić, V. Randić index and information. *AKCE Int. J. Graphs Comb.* **2018**, *15*, 307–312. [CrossRef]
6. Hosoya, H. Topological index, A newly proposed quantity characterizing the topological nautre of structural isomers of saturated hydrocarbons. *Bull. Chem. Soc. Jpn.* **1971**, *44*, 2332–2339. [CrossRef]
7. Hosoya, H. Clar's aromatic sextet and sextet polynomial. *Top. Curr. Chem.* **1990**, *153*, 255–272.
8. Farrell, E.J. An introduction to matching polynomials. *J. Comb. Theory* **1979**, *27*, 75–86. [CrossRef]
9. Gutman, I.; Hosoya, H. Molecular graphs with equal Zcounting and independence polynomials. *Z. Naturforsch.* **1990**, *45*, 645–648.
10. Gutman, I. Some analytical properties of the independence and matching polynomials. *Match Commun. Math. Comput. Chem.* **1992**, *28*, 139–150.
11. Stevanović, D.; Motoyama, A.; Hosoya, H. King and domino polynomials for polyomino graphs, Graph Theory Notes. *J. Math. Phys.* **1977**, *34*, 31–36.
12. Balasubramanian, K.; Ramaraj, R. Computer generation of king and color polynomials of graphs and lattices and their applications to statistical mechanics. *J. Comput. Chem.* **1985**, *6*, 447–454. [CrossRef]
13. Farrell, E.J.; De Matas, C.M. On star polynomials of complements of graphs. *Ark. Mat.* **1988**, *26*, 85–190. [CrossRef]
14. Farrell, E.J.; De Matas, C.M. Star polynomials of some families of graphs with small cyclomatic numbers. *Util. Math.* **1988**, *33*, 33–45.
15. Balasubramanian, K. On Graph Theoretical Polynomials in Chemistry. In *Mathematical and Computational Concepts in Chemistry*; Trinastic, N., Ed.; Ellis Horwood Ltd.: New York, NY, USA, 1986; pp. 20–33.

16. Dehmer, M.; Chen, Z.; Emmert-Streibd, F.; Mowshowitz, A.; Varmuzag, K.; Jodlbauer, H.; Shih, Y.; Tripathi, S.; Tao, J. The orbit-polynomial: A novel measure of symmetry in graphs. *IEEE Access* **2020**, *8*, 36100–36112. [CrossRef]
17. Dehmer, M.; Chen, Z.; Emmert-Streib, F.; Shi, Y.; Tripathi, S. Graph measures with high discrimination power revisited: A random polynomial approach. *Inform. Sci.* **2018**, *467*, 407–414. [CrossRef]
18. Balasubramanian, K.; Basak, S. C. Characterization of isospectral graphs using Ggraph invariants and derived orthogonal parameters. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 367–373. [CrossRef]
19. Dixon, J.D.; Mortimer, B. *Permutation Groups*; Springer: New York, NY, USA, 1996.
20. Harary, F. *Graph Theory*; Addison-Wesley Publishing Company: Boston, MA, USA, 1969.
21. Dehmer, M.; Mowshowitz, A.; Shi, Y. Structural differentiation of graphs using Hosoya-based indices. *PLoS ONE* **2014**, *7*, e102459. [CrossRef] [PubMed]
22. Dehmer, M.; Emmert-Streib, F.; Shi, Y. Graph distance measures based on topological indices revisited. *Appl. Math. Comput.* **2015**, *266*, 623–633. [CrossRef]
23. Mowshowitz, A.; Dehmer, M. The Hosoya entropy of a graph. *Entropy* **2015**, *17*, 1054–1062. [CrossRef]
24. Ghorbani, M.; Dehmer.; M.; Rajabi-Parsa, M.; Emmert-Streib, F.; Mowshowitz, A. Hosoya entropy of fullerene graph. *Appl. Math. Comput.* **2019**, *352*, 88–98.
25. Ghorbani, M.; Dehmer; Mowshowitz, A.; Emmert-Streib, F. The Hosoya entropy of graphs revisited. *Symmetry* **2019**, *11*, 1013. [CrossRef]
26. Ghorbani, M.; Dehmer.; M.; Cao, S.; Feng, L.; Tao, J.; Emmert-Streib, F. On the zeros of the partial Hosoya polynomial of graphs. *Inf. Sci.* **2020**, *524*, 199–215. [CrossRef]
27. Jachiymski, J. The contraction principle for mappings on a metric space with a graph. *Proc. Am. Math. Soc.* **2008**, 136, 1359–1373. [CrossRef]
28. Eskandar, A.; Aydi, H.; Arshad , M.; De la Sen, M. Hybrid Ćirić type graphic (Υ, Λ)-contraction mappings with applications to electric circuit and fractional differential equations. *Symmetry* **2020**, 12, 467.
29. Afshari, H.; Aydi, H.; Karapinar, E. On generalized α-ψ-Geraghty contractions on b-metric spaces. *Georg. J. Math.* **2020**, *27*, 9–21. [CrossRef]
30. Karapinar, E.; Czerwik, S.; Aydi, H. (α, ψ)-Meir-Keeler contraction mappings in generalized b-metric spaces. *J. Funct. Spaces* **2018**. [CrossRef]
31. Bollobás, B. *Random Graphs*, 2nd ed.; Cambridge Studies in Advanced Mathematics; Cambridge University Press: Cambridge, UK, 2001.
32. Bonchev, D.; Trinajestić, N. Information theory, distance matrix and molecular branching. *J. Chem. Phys.* **1977**, *67*, 4517–4533. [CrossRef]
33. Bonchev, D.; Rouvray, D.H. Introduction and Fundamentals. In *Chemical Graph Theory*; Abacus Press: New York, NY, USA, 1991.
34. Dehmer, M. Information processing in complex networks: Graph entropy and information functionals. *Appl. Math. Comput.* **2008**, *201*, 82–94. [CrossRef]
35. Rashevsky, N. Life, information theory, and topology. *Bull. Math. Biophys.* **1955**, *17*, 229–235. [CrossRef]
36. Mowshowitz, A. Entropy and the complexity of graphs: I. An index of the relative complexity of a graph. *Bull. Math. Biophys.* **1968**, *30*, 175–204. [CrossRef]
37. Gutman, I. The Energy of a Graph: Old and New Results. In *Algebraic Combinatorics and Applications*; Betten, A., Kohnert, A., Laue, R., Wassermann, A., Eds.; Springer: Berlin, Germany, 2001; pp. 196–211.