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Note

On the matching polynomial of subdivision graphs

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ABSTRACT

Let G be a simple graph and let $S(G)$ be the subdivision graph of G, which is obtained from G by replacing each edge of G by a path of length two. In this paper, by the Principle of Inclusion and Exclusion we express the matching polynomial and Hosoya index of $S(G)$ in terms of the matchings of G. Particularly, if G is a regular graph or a semi-regular bipartite graph, then the closed formulae of the matching polynomial and Hosoya index of $S(G)$ are obtained. As an application, we prove a combinatorial identity.

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1. Introduction

Throughout this paper, we suppose that G is a simple graph with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and the edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$, if not specified. Let A be a subset of the vertex set $V(G)$. By $G - A$ we denote the induced subgraph of G by deleting all vertices in A and the incident edges from G. For any arbitrary $v_i \in V(G)$, we use $d_G(i)$ (or d_i) to denote the degree of v_i. A set M of edges in G is a matching if every vertex of G is incident with at most one edge in M; it is a perfect matching if every vertex of G is incident with exactly one edge in M. Let $\mathcal{M}_i(G)$ denote the set of matchings of G with i edges. Hence $\mathcal{M}(G) = \mathcal{M}_0(G) \cup \mathcal{M}_1(G) \cup \cdots \cup \mathcal{M}_{\lfloor \frac{n}{2} \rfloor}(G)$ is the set of matchings of G. For an edge subset S of G, denote by $V(S)$ the set of vertices of G each of which is incident with at least one edge in S. Denote by $\phi_k(G)$ the number of matchings of G with k edges, that is, $\phi_k(G) = |\mathcal{M}_k(G)|$. We set $\phi_0(G) = 1$ by convention. Thus, if n is even, then $\phi_{\frac{n}{2}}(G)$ is the number of perfect matchings of G. The number of matchings of G is called the Hosoya index (see Hosoya [6]) and will be denoted by $Z(G)$, that is, $Z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} |\mathcal{M}_k(G)| = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \phi_k(G)$. The following two polynomials $m(G, x)$ and $g(G, x)$ are called the matching polynomial and the matching generating function of G, respectively (see [9]):

$$m(G, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k \phi_k(G) x^{n-2k} = \sum_{M \in \mathcal{M}(G)} (-1)^{|M|} x^{n-2|M|},$$

$$g(G, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \phi_k(G) x^k = \sum_{M \in \mathcal{M}(G)} x^{|M|}.$$

Hence we have

$$m(G, x) = x^n g(G, -x^{-2}), \qquad Z(G) = g(G, 1). \tag{1}$$

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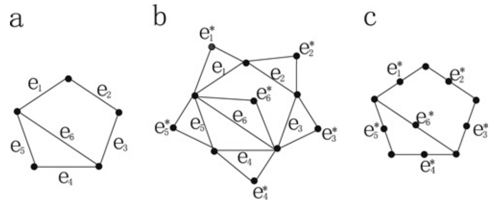

Fig. 1. (a) The graph G. (b) The graph operator $R(G)$ of G. (c) The subdivision graph $S(G)$ of G.

Obviously, the matching polynomial can be uniquely determined by the matching generating function, and vice versa.

The matching polynomial (or matching generating function) is a crucial concept in the topological theory of aromaticity [10]. The matching polynomial is also named the acyclic polynomial in [4,6,10]. Sometimes, the matching polynomial is also referred to as the reference polynomial [1]. It takes no great imagination to consider the idea of representing a molecule by a graph, with the atoms as vertices and the bonds as edges, but it is surprising that there can be an excellent correlation between the chemical properties of the molecule and suitably chosen parameters of the associated graph. One such parameter is the sum of the absolute values of the zeros of the matching polynomial of the graph, and this has been related to properties of aromatic hydrocarbons. The roots of the matching polynomial correspond to energy levels of a molecule and a reference structure. A new application in Hückel theory was discussed in detail in Trinajstić [11]. Hosoya [6] used the Hosoya polynomial in chemical thermodynamics. For further applications of the matching polynomial (or matching generating function) in chemistry, see for example the book [10] by Trinajstić. The computation of $Z(G)$ and $m(G, x)$ is NP-Complete [7]. For some related results see also [2,5,8,12–19].

Suppose G is a simple graph with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and the edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. Define two graph operators $R(G)$ and $S(G)$ (see the definitions in page 63 in Cvetković et al. [3]) as follows. Let $R(G) = (V(R(G)), E(R(G)))$ be the graph obtained from G by adding a new vertex e^* corresponding to each edge $e = (a, b) = ab$ of G and by joining each new vertex e^* to the end vertices a and b of the edge $e = (a, b)$ corresponding to it, that is, $R(G)$ is obtained from G by "changing each edge $e = ab$ of G into a triangle ae^*b". Hence $V(R(G)) = V(G) \cup \{e^*|e \in E(G)\}$ and $E(R(G)) = E(G) \cup \{(v_r, e^*), (v_s, e^*)|e = (v_r, v_s) \in E(G)\}$. Fig. 1(a) and (b) illustrate this procedure constructing $R(G)$ from G. Let $S(G)$ be the graph obtained from G by replacing each edge $e_i = (v_r, v_s)$ of G with a path $P(v_r - e_i^* - v_s)$ of length two. Hence $V(S(G)) = V(G) \cup \{e^*|e \in E(G)\}$ and $E(S(G)) = \{(v_r, e^*), (v_s, e^*)|e = (v_r, v_s) \in E(G)\}$. The graph $S(G)$ is called the subdivision graph of G. Fig. 1(a) and (c) illustrate this procedure constructing $S(G)$ from G.

In [14] we proved the following result:

Proposition 1.1 (*Yan and Yeh [14]*). *Let $G = (V(G), E(G))$ be a simple graph with n vertices and $R(G)$ the graph defined above. Then the Hosoya index $Z(R(G))$, or the number of matchings of $R(G)$, can be given by*

$$Z(R(G)) = (d_1 + 1)(d_2 + 1) \cdots (d_n + 1),$$

where $(d_1, d_2, \ldots, d_n)$ is the degree sequence of vertices of G.

In this paper, by the Principle of Inclusion and Exclusion we express the matching polynomial and the Hosoya index of the subdivision graph $S(G)$ of G in terms of the matchings of G. As applications, we prove that if G is a regular graph or a semi-regular bipartite graph then the matching polynomial and the Hosoya index of $S(G)$ can be determined uniquely by the matching numbers $\phi_i(G)$ for $0 \le i \le [\frac{n}{2}]$, where n is the number of vertices of G. Finally, we prove a combinatorial identity.

2. Main results

We first introduce the Principle of Inclusion and Exclusion. Let S be a finite set and $\omega : S \longrightarrow \mathcal{R}$ a weighted function, where $\mathcal{R}$ is a ring. For any subset S' of S, define $\omega(S')$ to be the summation of weights of elements of S'. Let $S_1, S_2, \ldots, S_r$ be the subsets of S (not necessarily distinct). For each subset T of $\{1, 2, \ldots, r\}$, let

$$S_T = \cap_{i \in T} S_i,$$

with $S_\emptyset = S$, and for $0 \le k \le r$ set

$$\omega(T_k) = \sum_{|T|=k} \omega(S_T).$$

Then

$$\omega(\bar{S_1} \cap \bar{S_2} \cap \cdots \cap \bar{S_r}) = \omega(T_0) - \omega(T_1) + \omega(T_2) + \cdots + (-1)^r \omega(T_r).$$

In order to formulate our main results, we need to introduce some terminology and notation as follows. Let G be a graph with vertex set $\{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$, and let $S(G)$ be the subdivision graph of G. Let E_i be

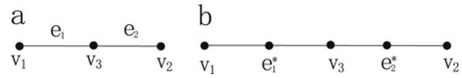

Fig. 2. (a) The graph G. (b) The subdivision graph $S(G)$ of G.

the set of all edges incident with vertex v_i in $S(G)$ for $1 \le i \le n$. Define N as the set of vectors $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n)$, the entries α_i of which are the subsets of E_i such that $|\alpha_i| \le 1$. That is,

$$N = \{(\alpha_1, \alpha_2, \ldots, \alpha_n) | \alpha_i \subset E_i \text{ and } |\alpha_i| = 0 \text{ or } 1 \text{ for } 1 \le i \le n\}.$$

Note that there exist exactly $d_G(i) + 1$ methods to choose α_i, i.e., α_i can be the empty set or any edge (set) incident with vertex v_i. Hence we have

$$|N| = \prod_{i=1}^{n} (1 + d_G(i)).$$

Let $Z[x]$ be the polynomial ring with integer coefficients and $\omega : N \longrightarrow Z[x]$ be a weighted function such that for any $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n) \in N$ we have $\omega(\alpha) = x^{\sum_{i=1}^{n} |\alpha_i|}$ (that is, α_i contributes one to $\omega(\alpha)$ if it is an empty set and contributes x to $\omega(\alpha)$ otherwise). Suppose that N' is a subset of N. Define $\omega(N')$ to be the summation of weights of elements in N' if $N' \ne \emptyset$ and $\omega(N') = 0$ otherwise. We use an example to explain the above definitions.

Let $G = (V(G), E(G))$ be the graph illustrated in Fig. 2(a), where $V(G) = \{v_1, v_2, v_3\}$ and $E(G) = \{e_1, e_2\}$. Hence the subdivision graph $S(G)$ of G (see Fig. 2(b)) has vertex set $V(S(G)) = \{v_1, v_2, v_3, e_1^*, e_2^*\}$ and edge set $E(S(G)) = \{v_1e_1^*, v_2e_2^*, v_3e_1^*, v_3e_2^*\}$. By the definition of N, we have

$$N = \{\beta_i | 1 \le i \le 12\},$$

where $\beta_1 = (\emptyset, \emptyset, \emptyset)$, $\beta_2 = (\emptyset, \emptyset, \{v_3e_1^*\})$, $\beta_3 = (\emptyset, \emptyset, \{v_3e_2^*\})$, $\beta_4 = (\emptyset, \{v_2e_2^*\}, \emptyset)$, $\beta_5 = (\{v_1e_1^*\}, \emptyset, \emptyset)$, $\beta_6 = (\emptyset, \{v_2e_2^*\}, \{v_3e_1^*\})$, $\beta_7 = (\emptyset, \{v_2e_2^*\}, \{v_3e_2^*\})$, $\beta_8 = (\{v_1e_1^*\}, \emptyset, \{v_3e_1^*\})$, $\beta_9 = (\{v_1e_1^*\}, \emptyset, \{v_3e_2^*\})$, $\beta_{10} = (\{v_1e_1^*\}, \{v_2e_2^*\}, \emptyset)$, $\beta_{11} = (\{v_1e_1^*\}, \{v_2e_2^*\}, \{v_3e_1^*\})$ and $\beta_{12} = (\{v_1e_1^*\}, \{v_2e_2^*\}, \{v_3e_2^*\})$. Furthermore, we can show that $\omega(N) = 1 + 4x + 5x^2 + 2x^3 = (1 + xd_G(v_1))(1 + xd_G(v_2))(1 + xd_G(v_3))$. This is not accidental. Generally, we have the following lemma:

Lemma 2.1. *Let G be a graph with vertex set $\{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$, and let $S(G)$ be the subdivision graph of G. Suppose that N and $\omega(N)$ are defined as above. Then*

$$\omega(N) = \prod_{i=1}^{n} (1 + xd_G(i)). \quad (2)$$

Proof. Let $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n) \in N$. Note that α_i can be the empty set or $\{v_ie_{i_k}^*\}$ for $1 \le k \le d_G(i)$, where $E_i = \{v_ie_{i_k}^* | 1 \le k \le d_G(i)\}$. Hence α_i contributes one to $\omega(\alpha)$ if α_i is the empty set and it contributes $x^{|\alpha_i|} = x$ to $\omega(\alpha)$ otherwise. Thus α_i contributes $1 + xd_G(i)$ to $\omega(N)$. Hence we have $\omega(N) = \prod_{i=1}^{n}(1 + xd_G(i))$. □

Let $e_i = (v_s, v_t) \in E(G)$ be an edge of G. Define N_i to be the subset of N such that, for any element $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n) \in N_i$, $\alpha_s = \{v_se_i^*\}$ and $\alpha_t = \{v_te_i^*\}$, respectively. That is, for an arbitrary edge $e_i = (v_s, v_t) \in E(G)$,

$$N_i = \{\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n) | \alpha \in N, \alpha_s = \{v_se_i^*\} \text{ and } \alpha_t = \{v_te_i^*\}\}.$$

Lemma 2.2. *Let G be a graph with vertex set $\{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$, and let $S(G)$ be the subdivision graph of G. Suppose that N_i is defined as above for $1 \le i \le m$. For $1 \le i_1 < i_2 < \cdots < i_k \le m$, let $M = \{e_{i_1}, e_{i_2}, \ldots, e_{i_k}\}$ be an edge subset of G.*

1. *If M is a matching of G, we have*

$$\omega(N_{i_1} \cap N_{i_2} \cap \cdots \cap N_{i_k}) = x^{2k} \prod_{v_j \in V(G) \setminus V(M)} (1 + xd_G(j));$$

2. *If M is not a matching, we have*

$$\omega(N_{i_1} \cap N_{i_2} \cap \cdots \cap N_{i_k}) = 0.$$

Proof. We first prove that $N_{i_1} \cap N_{i_2} \cap \cdots \cap N_{i_k} = \emptyset$ if $M = \{e_{i_1}, e_{i_2}, \ldots, e_{i_k}\}$ is not a matching of G. Note that if M is not a matching of G, then there exist at least two edges e_{i_s} and e_{i_t} in M such that $|V(e_{i_s}) \cap V(e_{i_t})| = 1$. Without loss of generality, suppose that $e_{i_s} = (v_a, v_b)$ and $e_{i_t} = (v_a, v_c)$, where $v_b \ne v_c$. By the definition of N_{i_s} and N_{i_t}, for arbitrary $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n) \in N_{i_s}$ and $\alpha' = (\alpha_1', \alpha_2', \ldots, \alpha_n') \in N_{i_t}$, we have $\alpha_a = \{v_ae_{i_s}^*\}$ and $\alpha_a' = \{v_ae_{i_t}^*\}$. If $N_{i_1} \cap N_{i_2} \cap \cdots \cap N_{i_k} \ne \emptyset$, then there exists at least a $\beta = (\beta_1, \beta_2, \ldots, \beta_n) \in N_{i_1} \cap N_{i_2} \cap \cdots \cap N_{i_k} \subseteq N_{i_s} \cap N_{i_t}$, i.e., $\beta \in N_{i_s}$ and $\beta \in N_{i_t}$. Hence $\beta_a = \{v_ae_{i_s}^*\} = \{v_ae_{i_t}^*\}$, a contradiction with $e_{i_s} \ne e_{i_t}$. Hence $\omega(N_{i_1} \cap N_{i_2} \cap \cdots \cap N_{i_k}) = 0$ if M is not a matching of G.

Now we prove the first statement. Let $e_{i_j} = (v_{a_j}, v_{b_j})$ for $1 \le j \le k$. If $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n) \in \cap_{j=1}^{k} N_{i_j}$, then $\alpha_{a_j} = \{v_{a_j} e^*_{i_j}\}$ and $\alpha_{b_j} = \{v_{b_j} e^*_{i_j}\}$ for $1 \le j \le k$. Furthermore, for arbitrary $\alpha_i \notin \{\alpha_{a_i} | 1 \le i \le k\} \cup \{\alpha_{b_i} | 1 \le i \le k\}$, $|\alpha_i|$ can be zero, which contributes $x^0 = 1$ to $\omega(\alpha)$, or $|\alpha_i|$ can be one, which contributes $x^1 = x$ to $\omega(\alpha)$. If M is a matching of G, then arbitrary two edges of $S(G)$ in $\{v_{a_j} e^*_{i_j} | 1 \le j \le k\} \cup \{v_{b_j} e^*_{i_j} | 1 \le j \le k\}$ are different. Hence $2k$ edges $v_{a_j} e^*_{i_j}$ and $v_{b_j} e^*_{i_j}$ for $1 \le j \le k$ contribute x^{2k} to $\omega(\alpha)$. With a similar reason as in the proof of Lemma 2.1, we have

$$\omega(N_{i_1} \cap N_{i_2} \cap \cdots \cap N_{i_k}) = x^{2k} \prod_{v_j \in V(G) \setminus V(M)} (1 + x d_G(j)).$$

The lemma thus follows. □

By the Principle of Inclusion and Exclusion, the following result is immediate from Lemmas 2.1 and 2.2.

Lemma 2.3. *Let G be a graph with vertex set $\{v_1, v_2, \dots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \dots, e_m\}$, and let $S(G)$ be the subdivision graph of G. Suppose that N and N_i are as in Lemma 2.2. Then we have*

$$\omega(\overline{N_1 \cup N_2 \cup \cdots \cup N_m}) = \sum_{M \in \mathcal{M}(G)} (-1)^{|M|} x^{2|M|} \left(\prod_{v_j \in V(G) \setminus V(M)} (1 + x d_G(j)) \right).$$

Now we can start to prove our main result.

Theorem 2.1. *Let G be a graph with vertex set $\{v_1, v_2, \dots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \dots, e_m\}$, and let $S(G)$ be the subdivision graph of G. Then*

$$m(S(G), x) = x^{m-n} \sum_{M \in \mathcal{M}(G)} (-1)^{|M|} \left(\prod_{v_j \in V(G) \setminus V(M)} (x^2 - d_G(j)) \right), \tag{3}$$

$$g(S(G), x) = \sum_{M \in \mathcal{M}(G)} (-1)^{|M|} x^{2|M|} \left(\prod_{v_j \in V(G) \setminus V(M)} (1 + x d_G(j)) \right), \tag{4}$$

where $m(G, x)$, $g(G, x)$, and $\mathcal{M}(G)$ are the matching polynomial, matching generating function of G, and the set of matchings of G, respectively.

Proof. Note that, by (1), (3) follows from (4). Hence we only need to prove that (4) holds. By Lemma 2.3, we need to prove the following (5) holds:

$$g(S(G), x) = \omega(\overline{N_1 \cup N_2 \cup \cdots \cup N_m}). \tag{5}$$

Let $N^\star$ be the set of edge subsets of $S(G)$, each of which has the form of $\alpha_1 \cup \alpha_2 \cup \cdots \cup \alpha_n$ for some $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n) \in \overline{N_1} \cap \overline{N_2} \cap \cdots \cap \overline{N_m}$. By the definition of N_i, $N^\star$ equals exactly the set $\mathcal{M}(S(G))$ of matchings of $S(G)$. Hence

$$\begin{aligned} g(S(G), x) &= \sum_{M \in \mathcal{M}(S(G))} x^{|M|} \\ &= \sum_{\cup_{i=1}^{n} \alpha_i \in N^\star} x^{\sum_{i=1}^{n} |\alpha_i|} \\ &= \sum_{\alpha \in \overline{N_1} \cap \overline{N_2} \cap \cdots \cap \overline{N_m}} x^{|\alpha|} \\ &= \sum_{\alpha \in \overline{N_1} \cap \overline{N_2} \cap \cdots \cap \overline{N_m}} \omega(\alpha) \\ &= \omega(\overline{N_1} \cap \overline{N_2} \cap \cdots \cap \overline{N_m}). \end{aligned}$$

Note that $\overline{N_1 \cup N_2 \cup \cdots \cup N_m} = \overline{N_1} \cap \overline{N_2} \cap \cdots \cap \overline{N_m}$. Hence (5) holds and we have finished the proof of the theorem. □

The following corollaries are immediate from Theorem 2.1:

Corollary 2.1. *Let G be a d-regular graph with n vertices and m edges and $S(G)$ the subdivision graph of G. Then*

$$m(S(G), x) = x^{m-n} m(G, x^2 - d), \qquad g(S(G), x) = (1 + xd)^n g\left(G, -\frac{x^2}{(1 + xd)^2}\right),$$

where $m(G, x)$ and $g(G, x)$ are the matching polynomial and matching generating function of G, respectively.

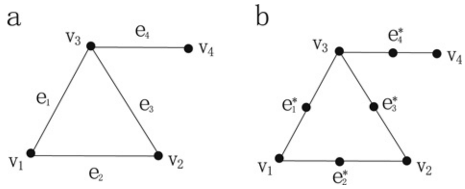

Fig. 3. (a) The graph G. (b) The subdivision graph $S(G)$ of G.

Corollary 2.2. *Let G be a (r_1, r_2) semi-regular bipartite graph with an (m, n)-bipartition ($m \le n$). Then*

$$m(S(G), x) = x^{mr_1-m-n} \sum_{i=0}^{m} (-1)^i \phi_i(G)(x^2 - r_1)^{m-i}(x^2 - r_2)^{n-i}; \tag{6}$$

$$g(S(G), x) = \sum_{i=0}^{m} (-1)^i \phi_i(G) x^{2i}(1 + r_1 x)^{m-i}(1 + r_2 x)^{n-i}. \tag{7}$$

Corollary 2.3. *Let G be a graph with vertex set $\{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$, and let $S(G)$ be the subdivision graph of G. Then*

$$Z(S(G)) = \sum_{M \in \mathcal{M}(G)} (-1)^{|M|} \left(\prod_{v_j \in V(G) \setminus V(M)} (1 + d_G(j)) \right).$$

Corollary 2.4. *Let G be a d-regular graph with n vertices and m edges and $S(G)$ the subdivision graph of G. Then*

$$Z(S(G)) = m(G, d + 1).$$

Corollary 2.5. *Let G be a (r_1, r_2) semi-regular bipartite graph with an (m, n)-bipartition ($m \le n$). Then*

$$Z(S(G)) = \sum_{i=0}^{m} (-1)^i \phi_i(G)(1 + r_1)^{m-i}(1 + r_2)^{n-i}.$$

Now we use an example to show how to use our main result. Let G be a graph with four vertices illustrated in Fig. 3(a). The subdivision graph of G is shown in Fig. 3(b). Note that G has six matchings: $\emptyset$, $\{e_1\}$, $\{e_2\}$, $\{e_3\}$, $\{e_4\}$ and $\{e_2, e_4\}$, where $\emptyset$ denotes the matching with no edge. That is, $\mathcal{M}(G) = \{\emptyset, \{e_1\}, \{e_2\}, \{e_3\}, \{e_4\}, \{e_2, e_4\}\}$. Hence, by Theorem 2.1, the matching polynomial of $S(G)$ is $m(S(G), x) = (x^2-1)(x^2-2)^2(x^2-3) - (x^2-1)(x^2-2) - (x^2-1)(x^2-3) - (x^2-1)(x^2-2) - (x^2-2)^2 + 1 = x^8 - 8x^6 + 19x^4 - 14x^2 + 2$.

Finally, we use Corollary 2.4 to prove a combinatorial identity. Let C_n be a cycle with n vertices. The subdivision graph of G is a cycle C_{2n} with $2n$ vertices. It is well known that $\phi_i(C_n) = \frac{n}{n-i}\binom{n-i}{i}$ for $1 \le i \le \lfloor \frac{n}{2} \rfloor$. Note that, by Corollary 2.4, we have $Z(C_{2n}) = m(C_n, 3)$. Hence we obtain the following:

Corollary 2.6. *Let n be a positive integer and $n \ge 3$. Then*

$$\sum_{i=0}^{n} \frac{2n}{2n-i} \binom{2n-i}{i} = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k \frac{n}{n-k} \binom{n-k}{k} 3^{n-2k}.$$

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