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HOSOYA AND MERRIFIELD-SIMMONS INDICES OF SOME CLASSES OF CORONA OF TWO GRAPHS

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Abstract. Let $G = (V, E)$ be a simple graph of order n and size m. An r-matching of G is a set of r edges of G which no two of them have common vertex. The Hosoya index $Z(G)$ of a graph G is defined as the total number of its matchings. An independent set of G is a set of vertices where no two vertices are adjacent. The Merrifield-Simmons index of G is defined as the total number of the independent sets of G. In this paper we obtain Hosoya and Merrifield-Simmons indices of corona of some graphs.

1. Introduction

Let $G = (V, E)$ be a simple graph of order n and size m. An r-matching of G is a set of r edges of G which no two of them have common vertex.
The Hosoya index $Z(G)$ of a graph G is defined as the total number of its matchings [8]. If $m(G, k)$ denotes the number of its k-matchings, then

$$Z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G, k).$$

The Hosoya index of a graph has application to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures.
An independent set of a graph G is a set of vertices where no two vertices are adjacent. The independence number is the size of a maximum independent set in the graph.

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The Merrifield-Simmons index of G is defined as the total number of the independent sets of G and denoted by $i(G)$. The Merrifield-Simmons index was introduced in 1982 in [10]. The Merrifield-Simmons index is one of the most popular topological indices in chemistry, which was extensively studied in a monograph [9]. There have been many papers studying the Merrifield-Simmons index (see [12, 14]).

Paper [11] obtain the Hosoya and Merrifield-Simmons indices for some classes of cartesian product of two specific graphs. In this paper we would like to obtain these indices for some classes of another product of two graphs.

The corona of two graphs G_1 and G_2, is the graph $G = G_1 \circ G_2$ formed from one copy of G_1 and $|V(G_1)|$ copies of G_2, where the ith vertex of G_1 is adjacent to every vertex in the ith copy of G_2 ([4]).

In this paper we investigate the Hosoya and Merrifield-Simmons indices for corona of some graphs. We denote the complete graph of order n and the complement of G, by K_n and $\overline{G}$, respectively.

2. Hosoya index of corona of two specific graphs

In this section, we will study Hosoya index of corona of some graphs. We use the following theorem to obtain main results.

Theorem 2.1. ([5, 7])

(i) *Let G be graph with k components $G_1, \ldots, G_k$, then*

$$Z(G) = \prod_{i=1}^{k} Z(G_i).$$

(ii) *Let G be a graph, and let $uv \in E(G)$. Then*

$$Z(G) = Z(G - uv) + Z(G - \{u, v\}).$$

Here we consider the corona of P_n and C_n with K_1. We denote $P_n \circ K_1$ and $C_n \circ K_1$ simply by P_n^* and C_n^*, respectively. See Figure 1. The following theorem gives the Hosoya index of $P_n \circ K_1$ and $C_n \circ K_1$.

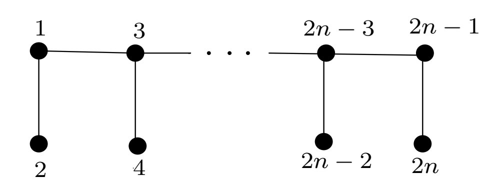

FIGURE 1. Labeled $P_n \circ K_1$.

Theorem 2.2. (i) *For every $n \geq 3$, $Z(P_n^*) = Z(P_n \circ K_1) = \frac{(1+\sqrt{2})^{n+1} - (1-\sqrt{2})^{n+1}}{2\sqrt{2}}$.*

(ii) *For every $n \geq 3$, $Z(C_n^*) = Z(C_n \circ K_1) = \frac{(2+\sqrt{2})(1+\sqrt{2})^{n-1} + (2-\sqrt{2})(1-\sqrt{2})^{n-1}}{\sqrt{2}}$.*

Proof.

(i) By Theorem 2.1(ii) we have $Z(P_n^*) = 2Z(P_{n-1}^*) + Z(P_{n-2}^*)$. The characteristic equation is $x^2 - 2x - 1 = 0$. So the roots of this equation are $1+\sqrt{2}$ and $1-\sqrt{2}$. Therefore the general solution is

$$Z(P_n^*) = c_1(1+\sqrt{2})^n + c_2(1-\sqrt{2})^n.$$

Now using initial values $Z(P_1^*) = Z(P_2) = 2$ and $Z(P_2^*) = Z(P_4) = 5$, we obtain

$$c_1 = \frac{1+\sqrt{2}}{2\sqrt{2}}, c_2 = \frac{\sqrt{2}-1}{2\sqrt{2}}.$$

So we have the result.

(ii) By Theorem 2.1 (ii) we have $Z(C_n^*) = Z(P_n^*) + Z(P_{n-2}^*) = 2(Z(P_{n-1}^*) + Z(P_{n-2}^*))$. Now we have the result by part (i). □

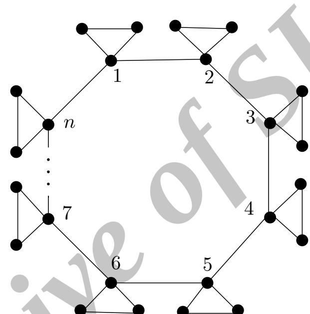

Figure 2. Graph $C_n \circ K_2$.

The following theorem gives us the Hosoya index of $P_n \circ K_2$ and $C_n \circ K_2$ (See Figure 2).

Theorem 2.3. ([3])

(i) *For every* $n \in \mathbb{N}$

$$Z(P_n \circ K_2) = \frac{2+\sqrt{2}}{4}(2+2\sqrt{2})^n + \frac{2-\sqrt{2}}{4}(2-2\sqrt{2})^n$$

(ii) *For every* $n \geq 3$

$$Z(C_n \circ K_2) = 2^n[(1+\sqrt{2})^n + (1-\sqrt{2})^n]$$

The following theorem is about the Hosoya index of graphs $P_n \circ \overline{K_i}$ and $C_n \circ \overline{K_i}$.

Theorem 2.4. *Suppose that* $i \in \mathbb{N}$ *and* $\alpha = i+1, \beta = \sqrt{\alpha^2+4}$. *Then*

(i) *For every* $n \in \mathbb{N}$,

$$Z(P_n \circ \overline{K_i}) = \frac{\alpha+\beta}{2\beta}(\frac{\alpha+\beta}{2})^n + \frac{\beta-\alpha}{2\beta}(\frac{\alpha-\beta}{2})^n.$$

(ii) *For every $n \geq 3$ and $i \in \mathbb{N}$,*

$$Z(C_n \circ \overline{K_i}) = \frac{1}{\beta}\left[(\frac{\alpha+\beta}{2})^{n+1} + (\frac{\alpha+\beta}{2})^{n-1} - (\frac{\alpha-\beta}{2})^{n+1} - (\frac{\alpha-\beta}{2})^{n-1}\right].$$

Proof. Let $G_n = P_n \circ \overline{K_i}$ .By the definition of Hosoya index and Lemma we have

$$\begin{aligned} Z(G_n) &= Z(P_n \circ \overline{K_i}) \\ &= Z(G_n - v_1v_2) + Z(G_n - \{v_1, v_2\}) \\ &= Z(G_1)Z(G_{n-1}) + Z(G_{n-2}) \\ &= (i+1)Z(G_{n-1}) + Z(G_{n-2}) \end{aligned}$$

In order to calculate $Z(G_n)$, we must provide the initial conditions. It is easy to arrive at that $Z(G_1) = i+1 = \alpha$, $Z(G_2) = (i+1)^2 + 1 = \alpha^2 + 1$. Thus, we the recurrence relation $Z(G_n) = (i+1)Z(G_{n-1}) + Z(G_{n-2})$ with initial conditions $Z(G_1) = i+1, Z(G_2) = (i+1)^2 + 1$.
The characteristic equation is $x^2 - (i+1)x - 1 = 0$. Using the quadratic formula, we find that the roots of this equation are

$$x_1 = \frac{(i+1) + \sqrt{(i+1)^2+4}}{2}, x_2 = \frac{(i+1) - \sqrt{(i+1)^2+4}}{2}$$

The general solution for the equation is

$$Z(G_n) = c_1(\frac{i+1+\sqrt{(i+1)^2+4}}{2})^n + c_2(\frac{i+1-\sqrt{(i+1)^2+4}}{2})^n$$

We would like to determine c_1 and c_2 that satisfy $Z(G_1) = i+1 = \alpha$ and $Z(G_2) = (i+1)^2+1 = \alpha^2+1$. By solving the system, we obtain $c_1 = \dfrac{\beta+\alpha}{2\beta}$, $c_2 = \dfrac{\beta-\alpha}{2\beta}$ Thus, we have the result. □

3. Merrifield-Simmons index of corona of two specific graphs

In this section we obtain the Merrifield-Simmons of corona of two specific graphs. We do this with two different approaches. First we need the following Theorem:

Theorem 3.1. *Let v be a vertex of a graph G. Then $i(G) = i(G - \{v\}) + i(G - N[v])$.*

Theorem 3.2. (i) $i(P_n \circ K_1) = \frac{2+\sqrt{3}}{2\sqrt{3}}(1+\sqrt{3})^n + \frac{\sqrt{3}-2}{2\sqrt{3}}(1-\sqrt{3})^n$.
(ii) $i(C_n \circ K_1) = \frac{9\sqrt{3}+16}{2\sqrt{3}}(1+\sqrt{3})^{n-3} + \frac{9\sqrt{3}-16}{2\sqrt{3}}(1-\sqrt{3})^{n-3}$.

Proof.

(i) Let $G_n = P_n \circ K_1$. By Theorem 3.1, we have

$$\begin{aligned} i(G_n) &= i(G_n - \{v_1\}) + i(G_n - N[v_1]) \\ &= i(P_1)i(G_{n-1}) + i(P_1)i(G_{n-2}) \\ &= 2(i(G_{n-1}) + i(G_{n-2})). \end{aligned}$$

The characteristic equation is $x^2-2x-2=0$. So the roots of this equation are $1+\sqrt{3}$ and $1-\sqrt{3}$. Therefore the general solution is

$$i(G_n)=c_1(1+\sqrt{3})^n+c_2(1-\sqrt{3})^n.$$

Now using initial values $i(G_1)=i(P_1^*)=i(P_2)=3$ and $i(G_2)=i(P_2^*)=i(P_4)=8$, we obtain

$$c_1=\frac{2+\sqrt{3}}{2\sqrt{3}},c_2=\frac{\sqrt{3}-2}{2\sqrt{3}}.$$

So we have the result.

(ii) Let $G_n=C_n\circ K_1$. By Theorem 3.1, we have

$$\begin{aligned} i(G_n) &= i(G_n-\{v_1\})+i(G_n-N[v_1]) \\ &= i(P_{n-1}\circ K_1)+i(P_{n-3}\circ K_1) \end{aligned}$$

Using Part (i) we will have the result. □

Theorem 3.3. ([13])

(i) $i(P_n\circ K_2)=\frac{21+5\sqrt{21}}{42}(\frac{3+\sqrt{21}}{2})^n+\frac{21-5\sqrt{21}}{42}(\frac{3-\sqrt{21}}{2})^n$.

(ii) $i(C_n\circ K_2)=$
$\frac{21+5\sqrt{21}}{14}(\frac{3+\sqrt{21}}{2})^{n-1}+\frac{21-5\sqrt{21}}{14}(\frac{3-\sqrt{21}}{2})^{n-1}+\frac{63+15\sqrt{21}}{14}(\frac{3+\sqrt{21}}{2})^{n-3}+\frac{63-15\sqrt{21}}{14}(\frac{3-\sqrt{21}}{2})^{n-3}$.

Here using independence polynomial of a graph we obtain the Merrifield-Simmons index of certain graphs. Let us to recall the definition of independence polynomial of a graph.

For a graph G, let i_k denote the number of independent sets of cardinality k in G ($k=0,1,...$). The independence polynomial of G is $I(G,x)=\sum_{k=0} i_k x^k$. It is easy to see that Merrifield-Simmons index of G, is equal with $I(G,1)$.

Gutman in [6] has proved the following theorem for independence polynomial of corona of two graphs:

Theorem 3.4. *$I(G\circ H,x)=(I(H,x))^n I(G,\frac{x}{I(H,x)})$, where $n=|V(G)|$.*

If we put $H=K_1$, $H=K_2$ and $H=\overline{K_i}$ in the above theorem, we have the following corollary:

Corollary 3.5. (i) *If $x\notin\{-1,0\}$, then $I(G\circ K_1,x)=I(G^*,x)=(1+x)^n I(G,\frac{x}{1+x})$.*

(ii) *If $x\notin\{\frac{-1}{2},0\}$, then $I(G\circ K_2,x)=(1+2x)^n I(G,\frac{x}{1+2x})$.*

(iii) *If $x\notin\{-1,0\}$, then for every $i\in\mathbb{N}$, we have $I(G\circ\overline{K_i},x)=(1+x)^{in} I(G,\frac{x}{(1+x)^i})$.*

Now the following corollary gives the relationship between Merrifield-Simmons indices of graphs $G\circ K_1$, $G\circ K_2$ and $G\circ\overline{K_i}$ with their independence polynomials at specific points.

Corollary 3.6. (i) $i(G\circ K_1)=2^n I(G,\frac{1}{2})$.

(ii) $i(G\circ K_2)=3^n I(G,\frac{1}{3})$.

(iii) $i(G\circ\overline{K_i})=2^{in} I(G,\frac{1}{2^i})$.

We need the following results to obtain more results on Merrifield-Simmons indices of some classes of graphs:

Theorem 3.7. ([1])

(i) $I(P_n,x) = \prod_{s=1}^{\lfloor \frac{n+1}{2} \rfloor} \left(2x+1+2x\cos\frac{2s\pi}{n+2}\right)$,

(ii) $I(C_n,x) = \prod_{s=1}^{\lfloor \frac{n}{2} \rfloor} \left(2x+1+2x\cos\frac{(2s-1)\pi}{n}\right)$.

Theorem 3.8. (i) $i(P_n \circ K_1) = 2^n \prod_{s=1}^{\lfloor \frac{n+1}{2} \rfloor} \left(2+\cos\frac{2s\pi}{n+2}\right)$,

(ii) $i(C_n \circ K_1) = 2^n \prod_{s=1}^{\lfloor \frac{n}{2} \rfloor} \left(2+\cos\frac{(2s-1)\pi}{n}\right)$,

(iii) $i(P_n \circ K_2) = 3^n \prod_{s=1}^{\lfloor \frac{n+1}{2} \rfloor} \left(\frac{5}{3}+\frac{2}{3}\cos\frac{2s\pi}{n+2}\right)$,

(iv) $i(C_n \circ K_2) = 3^n \prod_{s=1}^{\lfloor \frac{n}{2} \rfloor} \left(\frac{5}{3}+\frac{2}{3}\cos\frac{(2s-1)\pi}{n}\right)$.

(v) *For every* $n,i \in \mathbb{N}$, $i(P_n \circ \overline{K_i}) = 2^{in} \prod_{s=1}^{\lfloor \frac{n+1}{2} \rfloor} \left(1+\frac{1}{2^{i-2}}\cos^2\frac{s\pi}{n+2}\right)$.

(vi) *For every* $n,i \in \mathbb{N}$, $i(C_n \circ \overline{K_i}) = 2^{in} \prod_{s=1}^{\lfloor \frac{n}{2} \rfloor} \left(1+\frac{1}{2^{i-2}}\cos^2\frac{(s-\frac{1}{2})\pi}{n}\right)$.

Remark. Using the following identities ([2], p.64) the reader can check the equalities of Theorems 3.2, 3.3 and 3.8. For real numbers a, b and positive integer n,

$$a^n - b^n = \begin{cases} (a-b)\prod_{s=1}^{\frac{n-1}{2}} \left(a^2+b^2-2ab\cos\frac{2s\pi}{n}\right); & \text{if } n \text{ is odd,} \\ (a-b)(a+b)\prod_{s=1}^{\frac{n-2}{2}} \left(a^2+b^2-2ab\cos\frac{2s\pi}{n}\right); & \text{if } n \text{ is even.} \end{cases}$$

$$a^n + b^n = (a+b)\prod_{s=1}^{\lfloor \frac{n}{2} \rfloor} \left(a^2+b^2-2ab\cos\frac{(2s-1)\pi}{n}\right).$$

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