ON THE MERRIFIELD-SIMMONS INDEX AND GENERATING FUNCTIONS FOR THE GRAPHS OF THE STATE P_L (2, n)

by

Inci GULTEKIN* and Fatih CEVIK

Department of Mathematics, Faculty of Science, Atatürk University, Erzurum, Turkey

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In this study, we compute Merrifield-Simmons index of graphs which corresponds to P_L (2, n) by using the decomposition formula. Examination shows that Merrifield-Simmons index of certain classes of graphs deduce as a result in a difference equation. Further, the prominent formula for Merrifield-Simmons index of P_L (2, n) and generating function are found as a function of the number n of hexagons in the state of P_L (2, n). Also the relations formed for the (P_L (2, n, n)) graphs obtained by combining two P_L (2, n) with a certain angle between them are given.

Key words: *molecular graph, Fibonacci number, decomposition formula, difference equation, generating function*

Introduction

Graph theory is one of the fastest growing topics and most popular subjects in mathematics since they have many up-to date applications in several area of science. Thus many researchers studied interdiciplinary relationship and as well as connections between such as number theory and also developed many interrelation properties. The area is active research area and many study many aspect of graphs and further properties of numbers with graphs. Let $G = (V, E)$ be a simple graph, where V is the set of its vertices and E is the set of its edges. Since the Fibonacci number of a graph is the number of independent vertex subsets that is for a graph G, when no two vertices from U are adjacent in G, the number of independent vertex subsets U of V is referred to as the consept of the Fibonacci number of an undirected graph $G = (V, E)$. The undirected simple graphs, which are graphs that do not have loops and multiple edge, we examined in this contribution. For further details, any of standard monographs, *e.g.* [1] may be referred to for the general graph-theoretic terminology.

Let F_n and L_n denote the n^{th} Fibonacci number and Lucas number, respectively. The well-known Fibonacci numbers F_n are defined by the second order recurrence $F_{n+2} = F_{n+1} + F_n$ with $F_0 = 0$, $F_1 = 1$. The same recurrence is satisfied by (the Lucas numbers) with the initial terms $L_0 = 2$, $L_1 = 1$. Fibonacci numbers F_{n+2} is the total of subsets of $\{1, 2, 3, \quad, n\}$ when no element are adjacent. The notion of the Fibonacci number of graph was introduced by Prodinger and Tichy [2] in 1982 on this view. On the other side the Merrifield-Simmons index or also known as σ-index and the Hosoya index or Z-index of a graph are two well known and prominent examples of topological indices which are of interest in combinatorial chemistry,

* Corresponding author, e-mail: igultekin@atauni.edu.tr

[3]. They are defined as the total number of independent vertex subsets as in the following definition and consider the total number of matchings of a graph, see for details [4-6].

Definition 1. The Merrifield-Simmons index of a graph $G = (V, E)$ is defined as the total numbers of all subsets U of V in which there is no two vertices in U that are adjacent [7].

The k-independent set of G is the subset U of k mutually independent vertices. The number of the k independent set of G is denoted as $i(G, k)$. By definition $i(G, 0) = 1$ for any graph G. Then the relation $\sigma(G) = \Sigma i(G, k)$ where the summation is taken over all non-negative integers k, [8].

We note that in the present study we use similar terminology and notation as in the [8], however we consider two adjacent four-membered rings approach. Thus, we obtain formula for the Fibonacci numbers of linear phenylenes and generating function that were found as a function of the number of hexagons in the phenylene by using the decomposition formulas.

Theorem 1. Let γ and δ be the distinct solutions of the equation $x^2 - ax - b = 0$ where $a, b \in \mathbb{R}$ and $b \neq 0$. Then every solution of linear homogenous recurrence relation with constant coefficients $a_n = aa_{n-1} + ba_{n-2}$ where $a_0 = C_0$ and $a_1 = C_1$ is of the form $a_n = A\gamma^n + B\delta^n$ for some constant A and B, [9].

Theorem 2. If $G_{1,}$ G_1, G_2 are disjoint graphs, then $f(G_1 \cup G_2) = f[(G_1) f(G_2)]$, [8].

Theorem 3. Let P_n be a path with n vertices and C_n a circuit with n vertices. Then $\sigma(P_n) = F_{n+2}$ and $\sigma(C_n) = L_n$, [7].

Theorem 4. Given that G is a graph with at least two vertices. The $v$shows the arbitrary vertex of graph G. Moreover $G - v$ is the subgraph of graph G that is obtained by deleting the vertex v from the graph G. Beside $G - (v)$ is also a subgraph of graph G that is obtained by deleting the vertex v and all the vertices adjacent to v. By using these subgraphs, the equation of $\sigma(G)$ is written as $\sigma(G) = \sigma(G - v) + \sigma[G - (v)]$, [7].

Theorem 5. If vertices u, v are adjacent in a graph G then $\sigma(G) = \sigma(G - uv) - \sigma(G - (u, v))$, where $G - uv$ is the subgraph of G obtained by deletion of the edge uv of G and $G - (u, v)$ is the subgraph of graph G obtained by deletion of the vertices u, v and all the vertices adjacent to them, [10].

In mathematical chemistry, a molecular graph is the presentation of the structural formula of a chemical compotent in terms of graph theory. In there, the Fibonacci numbers of a graph are expresed by Merrifield and Simmond index [2]. The fact that $\sigma(P_n)$ is always a Fibonacci number is also the reason why the number of independent set was called Fibonacci number of a graph by Prodinger and Tichy in [2]. Further, Prodinger and Tichy derived some basic and effective result for the Fibonacci numbers $f(G)$ of a graph $G = (V, E)$ [2].

In phenylenes each four-membered ring is adjacent to two 6-membered rings, and no two 6-membered rings are adjacent. Seibert and Koudela [8] calculated The Fibonacci numbers of molecular grahps corresponding to one type of phenylenes. By with the decomposition theorem used here, they introduced the subgrahps of these molecular grahps of one type of phenylenes and obtained system of difference equation.

In this study, we are concerned with the system named as $P_L(2, n)$, in which there are two adjacent four-membered rings that are adjacent to two six-membered rings, and no two six-membered rings are adjacent. Then we established the equation systems of Merrifield-Simmons indexes from the graphs corresponding to graph $P_L(2, n)$ and its subgraphs. Also we have obtained the recurrence relations and generating functions of the system by expressing the moletcular graphs with Merrifield-Simmons index for the state $P_L(2, n)$.

Main results

In this section, at first, we will find the equation systems of Merrifield-Simmons indexes from the graphs corresponding to graph $P_L(2, n)$ and its subgraphs $P_A(2, n)$, $P_B(2, n)$, $P_D(2, n)$, and $P_E(2, n)$ by using the appropriate decomposition theorem. Now, we will derive some results to Merrifield-Simmons index for $P_L(2, n)$. Then we consider $P_L(2, n)$ and its subgraphs $P_A(2, n)$, $P_B(2, n)$, $P_D(2, n)$, and $P_E(2, n)$, fig. 1.

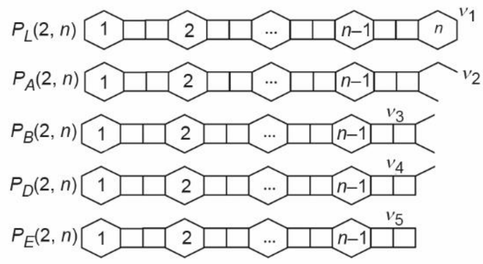

Figure 1. The graph of $P_L(2, n)$ and its subgraphs

The following formulas were derived from *Theorem 4* by suitable choces of the vertex v in the particular cases.

Lemma 1. Let $P_L(2, n)$ be the graph, in which there are two adjacent four-membered rings that are adjacent to two six-membered rings, and no two six-membered rings are adjacent with n hexagons and let $P_A(2, n)$, $P_B(2, n)$, $P_D(2, n)$, and $P_E(2, n)$ be graphs as in fig. 1. Then the following relations hold for any positive integer $n > 1$.

(i) $\sigma[P_L(2,n)] = \sigma[P_A(2,n)] + \sigma[P_D(2,n)]$
(ii) $\sigma[P_A(2,n)] = \sigma[P_B(2,n)] + \sigma[P_D(2,n)]$
(iii) $\sigma[P_B(2,n)] = 8\sigma[P_L(2,n-1)] + 12\sigma[P_A(2,n-1)]$
(iv) $\sigma[P_D(2,n)] = 5\sigma[P_L(2,n-1)] + 7\sigma[P_A(2,n-1)]$
(v) $\sigma[P_E(2,n)] = 3\sigma[P_L(2,n-1)] + 4\sigma[P_A(2,n-1)]$

Proof. If the removed vertex v is chosen in a suitable way, we can derive each relation by using *Theorem 4*, fig. 1. Specifically we choose vertex;

(i) v_1 in the n^{th} hexagon to obtain $\sigma[P_L(2,n)]$. $P_L(2,n) - v_1$ is the subgraph $P_A(2,n)$ of graph $P_L(2,n)$ that is obtained by deleting the vertex v_1 from the graph $P_L(2,n)$. Beside $P_L(2,n) - (v_1)$ is also a subgraph $P_D(2,n)$ of graph $P_L(2,n)$ that is obtained by deleting the vertex v_1 and all the vertices adjacent to v_1. By using these subgraphs, the equation of $\sigma(G)$ is written as $\sigma[P_L(2,n)] = \sigma[P_A(2,n)] + \sigma[P_D(2,n)]$

(ii) v_2 to obtain $\sigma[P_A(2,n)]$

(iii) v_3 of third degree that is on the last square and then we use again *Theorem 4* on the graph $P_B(2,n) - (v)$ and *Theorem 4*, with the fact that $\sigma(P_n) = F_{n+2}$, which gives desired expression,

(iv) v_4 in the last square and after that we use again *Theorem 4* on the graph $P_D(2,n) - v$ where the vertex of degree 1 is chosen,

(v) v_5 to one of vertices of third degree in the last square to obtain $\sigma[P_E(2,n)]$.

Relations (i)-(v) are also valid for $n > 1$, as the Fibonacci number of the empty graphs is equal to one. Let us denote topological indices of $\sigma[P_L(2,n)] = l_n$, $\sigma[P_A(2,n)] = a_n$, $\sigma[P_B(2,n)] = b_n$, $\sigma[P_D(2,n)] = d_n$, and $\sigma[P_E(2,n)] = e_n$ for short. We can obtain the values of these indices for the small numbers of n by using of *Theorem 4*. These values are collected in tab. 1.

Table 1. Merrifield-Simmons index of the graph $P_L(2, n)$ and its subgraphs

n	l_n	a_n	b_n	d_n	e_n
1	18	13	8	5	3
2	662	481	300	181	106
3	24422	17745	11068	6677	3910
4	900966	654641	408316	246325	144246

Next we have the following theorems for related expressions.

Theorem 6. $\sigma[P_A(2,n)]$ is expressed in the form:

$$\sigma[P_A(2,n)] = a_n = 13\left[\frac{x_1^n - x_2^n}{x_1 - x_2}\right]$$

for any $n \in \mathbb{Z}^+$, where $x_{1,2} = (37 \mp \sqrt{1353})/2$.

Proof. First of all, we will find a linear difference equation arising from *Lemma 1* with a_n as the unknown variable. If we add eqs. of (iii) and (iv) we can change the form of the system of relations which are:

$$b_n + d_n = 19a_{n-1} + 13l_{n-1} \tag{1}$$

from eq. (ii).

We can rewrite the system by using the reformed format of eq. (ii), as previously stated, then the equality (1) is regulated:

$$a_n = 13l_{n-1} + 19a_{n-1}$$

then the equation is regulated:

$$l_{n-1} = \frac{1}{13}a_n - \frac{19}{13}a_{n-1}$$

the equation is regulated where $n+1$ is written instead of n:

$$l_n = \frac{1}{13}a_{n+1} - \frac{19}{13}a_n \tag{2}$$

If we reform eqs. (*i*) and (*ii*):

$$l_n + b_n = 2a_n$$

and use eqs. (iii) and (2):

$$2a_n = \frac{1}{13}a_{n+1} - \frac{19}{13}a_n + 8l_{n-1} + 12a_{n-1}$$

$$26a_n = a_{n+1} - 19a_n + 104\left(\frac{1}{13}a_n - \frac{19}{13}a_{n-1}\right) + 156a_{n-1}$$

$$37a_n = a_{n+1} + 4a_{n-1}$$

Now replace n by $n+1$ then we obtain:

$$a_{n+2} - 37a_{n+1} + 4a_n = 0 \tag{3}$$

for any positive integer n. This equation is a homogenous linear difference equation of second order with constant coefficients. The corresponding characteristic equation is $x^2 - 37x + 4 = 0$ with two real roots. The roots of this equation are $x_{1,2} = (37 \mp \sqrt{1353})/2$. Then the general solution of eq. (3) is:

$$a_n = K_1 x_1^n + K_2 x_2^n \quad a_1 = 13, \quad a_2 = 481$$

for some constants K_1 and K_2. If the equations are solved in the statements a_2 and a_2

Then, $K_1 = 13/(x_1 - x_2)$ and $K_2 = 13/(x_2 - x_1)$ and its general solution becomes:

$$a_n = 13\left(\frac{x_1^n - x_2^n}{x_1 - x_2}\right)$$

Theorem 7. $\sigma[P_L(2,n)]$ is expressed in the form:

$$\sigma[P_L(2,n)] = l_n = \frac{1}{x_1 - x_2}[x_1^{n-1}(18x_1 - 4) + x_2^{n-1}(-18x_2 + 4)]$$

for any $n \in \mathbb{Z}^+$.

Proof. Since $l_n = (a_{n+1} - 19a_n)/13$ and $a_n = 13[(x_1^n - x_2^n)/(x_1 - x_2)]$ then by using the equations $x_1 + x_2 = 37$ and $x_1.x_2 = 4$ that are obtained from the equation $x^2 - 37x + 4 = 0$ the expression is obtained:

$$l_n = \frac{1}{x_1 - x_2}(x_1^{n+1} - x_2^{n+1} - 19x_1^n + 19x_2^n) = \frac{1}{x_1 - x_2}[x_1^{n-1}(x_1^2 - 19x_1) - x_2^{n-1}(x_2^2 - 19x_2)]$$

where $x_1^2 = 37x_1 - 4$ and $x_2^2 = 37x_2 - 4$ are written and the expression is regulated:

$$l_n = \frac{1}{x_1 - x_2}[x_1^{n-1}(18x_1 - 4) + x_2^{n-1}(-18x_2 + 4)]$$

we can give b_n, d_n, and e_n values in the following form for any $n \in \mathbb{Z}^+$:

$$\sigma[P_B(2,n)] = b_n = \frac{4}{x_1 - x_2}[x_1^{n-2}(75x_1 - 8) - x_2^{n-2}(75x_2 - 8)]$$

$$\sigma[P_D(2,n)] = d_n = \frac{1}{x_1 - x_2}[x_1^{n-2}(181x_1 - 20) - x_2^{n-2}(181x_2 - 20)]$$

$$\sigma[P_E(2,n)] = e_n = \frac{1}{x_1 - x_2}[x_1^{n-2}(106x_1 - 12) - x_2^{n-2}(106x_2 - 12)]$$

Next we give the ordinary generating functions for the sequences of the Fibonacci numbers of the graphs mentioned above by a classical way. The generating functions for the sequences $\{a_n\}$, $\{l_n\}$,$\{b_n\}$,$\{d_n\}$, and $\{e_n\}$ are in the form:

$$g_a(x)=\frac{13x}{1-37x+4x^2}$$

$$g_l(x)=\frac{18x-4x^2}{1-37x+4x^2}$$

$$g_b(x)=\frac{8x+4x^2}{1-37x+4x^2}$$

$$g_d(x)=\frac{5x-4x^2}{1-37x+4x^2}$$

$$g_e(x)=\frac{3x-5x^2}{1-37x+4x^2}$$

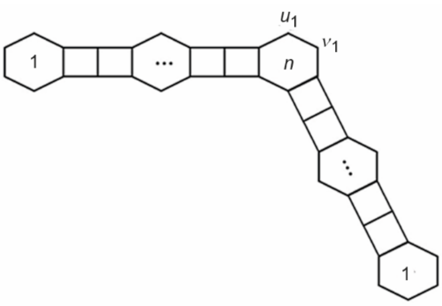

Figure 2. The molecular graph of $[P_L(2, n, n)]$

In addition to the *Lemma 1* results, the relations formed for the $[P_L(2,n,n)]$ graphs, fig. 2 obtained by combining two $P_L(2, n)$ with a certain angle between them are given in the following lemmas and theorems.

Lemma 2. The terms of the sequence $\sigma[P_L(2,n,n)]$ satisfy the relation:

$$\sigma[P_L(2,n,n)]=d_n^2-7l_{n-1}^2-12a_{n-1}^2-18l_{n-1}a_{n-1}$$

for any positive integer $n\geq 2.$.

Proof. If we choose the edge u_1v_1 in graph of $[P_L(2,n,n)]$ and use the *Theorem 5* then we are obtain $[P_L(2,n,n)]-u_1v_1$ and $[P_L(2,n,n)]-(u_1,v_1)$, fig. 3. Over again we choose the edge u_2v_2 in graph of $[P_L(2,n,n)]-u_1v_1$ and the edge u_3v_3 in graph of $[P_L(2,n,n)]-(u_1,v_1)$ and use the *Theorem 5*. Thus we have successively:

$$\sigma[P_L(2,n,n)]=\sigma[P_L(2,n,n)-u_1v_1]-\sigma[P_L(2,n,n)-(u_1,v_1)]=$$

$$=\sigma\{[P_L(2,n,n)-u_1v_1]-u_2v_2\}-\sigma\{P_L[(2,n,n)-u_1v_1]-(u_{2,}v_2)\}-$$

$$-\sigma\{[P_L(2,n,n)-(u_1,v_1)]-u_3v_3\}-\sigma\{[P_L(2,n,n)-(u_1,v_1)]-(u_3,v_3)\}$$

$$=d_n^2-7(l_{n-1}+a_{n-1})^2-4(l_{n-1}+a_{n-1})a_{n-1}-a_{n-1}^2$$

$$=d_n^2-7l_{n-1}^2-12a_{n-1}^2-18l_{n-1}a_{n-1}$$

Which gives the desired result.

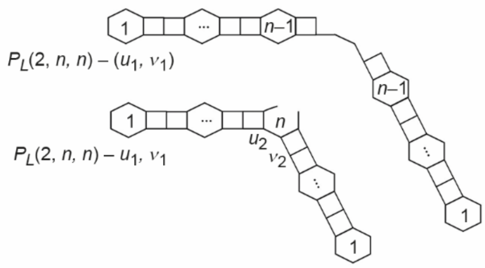

Figure 3. Subgraphs of graph [*P*$_L$(2, *n*, *n*)]

Theorem 8. $\sigma[P_L(2,n,n)]$ for any $n \in \mathbb{Z}^+$ can be written in the form:

$$\sigma[P_L(2,n,n)] = \frac{1}{(x_1 - x_2)^2}[(892065x_1 - 96724)x_1^{2n-4} + (892065x_2 - 96724)x_2^{2n-4} + 1352.4^{n-2}]$$

Proof. If we use *Lemma 2* and the given formulas l_n, a_n and d_n then we can easily and each the result

For any positive integer $n \geq 2$:

$$\sigma[P_L(2,n,n)] = \frac{1}{(x_1 - x_2)^2}[(181x_1 - 20)x_1^{n-2} - (181x_2 - 20)x_2^{n-2}]^2 -$$
$$-7[(18x_1 - 4)x_1^{n-2} - (18x_2 - 4)x_2^{n-2}]^2 - 12[13(37 - x_2)x_1^{n-2} - (37 - x_1)x_2^{n-2}]^2 -$$
$$-18\left[13\left(\left(37 - x_2\right)x_1^{n-2} - (37 - x_1\right)x_2^{n-2}\right)\left(\left(18x_1 - 20\right)x_1^{n-2} - (18x_2 - 20\right)x_2^{n-2}\right)\right]\}$$

$$\sigma[P_L(2,n,n)] = \frac{1}{(x_1 - x_2)^2}(1204917x_1 - 130644)x_1^{2n-4} + 4992.4^{n-2} +$$
$$+\left(1204917x_2 - 130644\right)x_1^{2n-4} + +(-82908x_1 + 8960)x_1^{2n-2} - 18928.4^{n-2} +$$
$$+\left(-82908x_2 + 8960\right)x_2^{2n-4} + \left(-75036x_1 + 8112\right)x_1^{2n-4} + 16224.4^{n-2} +$$
$$\left(-75036x_2 + 8112\right)x_1^{2n-4} + \left(-154908x_1 + 16848\right)x_1^{2n-4} +$$
$$+4.4^{n-2} + \left(-154908x_2 + 16848\right)x_2^{2n-4}$$

$$\sigma[P_L(2,n,n)] = \frac{1}{(x_1 - x_2)^2}\left[\left(892065x_1 - 96724)x_1^{2n-4} + (892065x_2 - 96724\right)x_2^{2n-4} + 1352.4^{n-2}\right]$$

Conclusion

In the present study, a difference equation of a higher order and a system of difference equations are obtained by using *Theorem 4* and we applied *Theorem 4* in order to find explicit fomulas, which depend on one or two parametres of Merrifield-Simmons index for various classes of graphs. The prominent formula for Merrifield-Simmons index of the state $P_L(2, n)$ and generating function are found as a function of the number n of hexagons in the state $P_L(2, n)$ by using the decomposition formulas.

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