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Computing the Number of k-Matchings in Benzenoid Chains

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Abstract

The Hosoya index is associated with many thermodynamic properties such as boiling point, entropy, total π-electron energy. Transfer matrix technique is extensively utilized in mathematical chemistry for various enumeration problems. In this paper, we introduce the k-matching vector at a certain edge of graph G. Then by using the k-matching vector and two recurrence formulas, we get reduction formulas to compute k-matching number $p(G,k)$ of any benzenoid chains for $\forall k \geq 0$ whose summation gives the Hosoya index of the chain. In conclusion, we compute $p(G,k)$ of any benzenoid chains via an appropriate multiplication of three $4(k+1)\times 4(k+1)$ dimensional transfer matrices and a terminal vector which can be obtained by given two algorithms.

1 Introduction

Let $G=(V,E)$ be a graph. A matching in G is a set of independent edges such that no two edges have a common vertex. A matching containing k independent edges is called a k-matching. Maximum possible number of k-matching in G is called k-matching number and it is denoted by $p(G,k)$, for some results about k-matching number (for $0 \leq k \leq 6$) of certain graphs see [1, 7, 8, 18, 19]. Relatedly, Hosoya index (Z index) of G is defined as the sum of all $p(G,k)$ in G, where $p(G,0)=1$, and it is denoted by $Z(G)=\sum_{k=0}^{r} p(G,k)$, where $p(G,r) \neq 0$ whereas $p(G,r+1)=0$, for details, see [12]. Hosoya index has significant importance and therefore, is extensively studied in mathematical chemistry to determine and quantify physical and structural properties of organic molecules, see for more details [9, 20].

Benzenoid (hexagonal) systems are graph forms of benzenoid hydrocarbons that have practical role in theoretical chemistry. A benzenoid system is represented as a finite 2-connected graph whose regions are hexagons excluding exterior region. Inner dual of a benzenoid system G is defined as a graph G' that each hexagon of G is represented as a vertex in G' and if two hexagons are adjacent in G, then corresponding vertices are adjacent in G'. A cata-condensed hexagonal system G is a hexagonal system that G' is a tree, for more information and research, see [10]. If every hexagon adjacent at most two hexagon in a cata-condensed hexagonal system, then it is called a hexagonal chain. Extremal properties of hexagonal chains were studied in [5, 11, 22].

Some studies on the number of k-matchings of specific molecular graphs can be found in [2, 3, 21]. In [15], Klabjan and Mohar presented a way to compute the number of k-matchings in hexagonal systems for $k \leq 5$.

In chemical graph theory, graph-theoretical and combinatorial enumeration problems can be solved by using recurrence relations repeatedly. However, these ways are often quite challenging to apply even with a computer for large and complex systems such as polycyclic graphs [4, 17]. At this point, two efficient and practical methods were presented by Hosoya and Ohkami [13], Randić et al. [17] to surpass these challenges that are called operator technique and transfer matrix technique, respectively. In [13], Hosoya and Ohkami obtained the recurrence equations of characteristic, matching and Z-counting polynomials for linear, kinked and zig-zag types polyacenes by using the operator technique. Furthermore, the operator technique was used in the study on some periodic lattice spaces by Hosoya and Motoyama, for details see [14]. In [17], Randić et al. proposed an algorithm in which they obtain the matching polynomials of any benzenoid chains via a product of three 5×5 dimensional transfer matrices with an appropriate terminal vector. With this technique, they also studied the number of Kekulé structures, the Hosoya indices and characteristic polynomials of arbitrary benzenoid chains. Analogously in [16], Polansky et al. computed the Wiener numbers of arbitrary benzenoid chains by using three 5×5 dimensional transfer matrices and an appropriate terminal vector. Moreover, in the same paper, it was shown that the Wiener numbers of large benzenoid systems are accessible by using various dimensional augmented transfer matrices.

In the transfer matrix technique [16, 17], a vector v is defined by associated with the corresponding benzenoid system with h hexagons. The desired value is represented in an entry of v. By multiplying v with an appropriate transfer matrix, the desired value for the benzenoid system with $h+1$ hexagons is achieved. In this technique, the defined vector is designed according to the corresponding benzenoid system. Also, each transfer matrix is obtained according to edge deletion operations to annihilate a hexagon in the corresponding benzenoid system.

In [6], R. Cruz et al. presented a method to compute the Hosoya index of a given cata-condensed hexagonal system by introducing a Hosoya vector and using the transfer matrix technique. As a sequel of the papers [6, 15, 17], first of all we introduce a $4(k+1) \times 1$ dimensional vector at an edge of a hexagon of a given benzenoid chain that we call as k-matching vector. After that, by using this vector and two significant recurrence formulae, we present reduction formulae to compute $p(G, k)$ of the benzenoid chain via an appropriate multiplication of three $4(k+1) \times 4(k+1)$ dimensional transfer matrices and a terminal vector where $k \geq 0$.

2 Computation of *k*-matchings in benzenoid chains

The most important recurrence formula to calculate the k-matching number of a graph G is as follows:

$$p(H \cup S, k) = p(H, k)p(S, 0) + p(H, k-1)p(S, 1) + \cdots + p(H, 1)p(S, k-1) + p(H, 0)p(S, k), \tag{1}$$

where $G = H \cup S$ and H, S are two connected components of G.

$$p(G, k) = p(G - e, k) + p(G - a - b, k - 1) \tag{2}$$

for an edge $e = ab$, see [13]. In the next definition, we present a k-matching vector of a graph G at a given edge to compute $p(G, k)$ of G.

Definition 2.1. *Let G be a graph and ab be an edge of G. The k-matching vector of G at the edge ab is defined as*

$$p_{ab}(G,k) = \begin{pmatrix} p(G,k) \\ p(G,k-1) \\ \vdots \\ p(G,1) \\ p(G,0) \\ p(G-a,k) \\ p(G-a,k-1) \\ \vdots \\ p(G-a,1) \\ p(G-a,0) \\ p(G-b,k) \\ p(G-b,k-1) \\ \vdots \\ p(G-b,1) \\ p(G-b,0) \\ p(G-a-b,k) \\ p(G-a-b,k-1) \\ \vdots \\ p(G-a-b,1) \\ p(G-a-b,0) \end{pmatrix}.$$

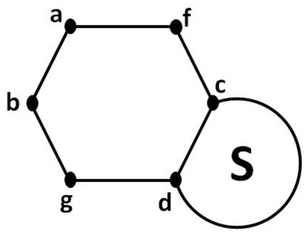

Figure 1. The graph in Thms. 2.1 and 2.3

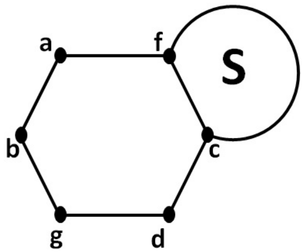

Figure 2. Graph in Thm. 2.2

Theorem 2.1. *Let $G = (V, E)$ be a graph derived from the edge-coalescence of the graph S and a hexagon at the edge cd of S (See Fig. 1). Then*

$$p_{ab}(G,k) = Q \cdot p_{cd}(S,k)$$

where the transfer matrix Q is a $4(k+1) \times 4(k+1)$ dimensional matrix as follows:

$$
\left(\begin{array}{cccccc|cccccc|cccccc|ccccccc}
1 & 3 & 1 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 0 & \cdots & 0 \\
0 & 1 & 3 & 1 & \cdots & 0 & 0 & 0 & 1 & 2 & \cdots & 0 & 0 & 0 & 1 & 2 & \cdots & 0 & 0 & 0 & 0 & 1 & 1 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 3 & 1 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & 0 & \cdots & 0 & 1 & 2 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\
0 & \cdots & 0 & 0 & 1 & 3 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\hline
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\
0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\hline
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\
0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\hline
1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\
0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0
\end{array}\right).
$$

Proof. First of all, we deal with the calculation of $p(G,k)$, $p(G-a,k)$, $p(G-b,k)$ and $p(G-a-b,k)$ by deleting the edges gd and cf. Subsequently, we use the recurrence relations 1 and 2 as follows:

$$
\begin{aligned}
p(G,k) &= p(G-gd-cf,k) + p(G-gd-c-f,k-1) + p(G-g-d-cf,k-1) \\
&\quad + p(G-g-d-c-f,k-2) = p(S\cup P_4,k) + p((S-c)\cup P_3,k-1) \\
&\quad + p((S-d)\cup P_3,k-1) + p((S-c-d)\cup P_2,k-2) \\
&= p(S,k) + 3p(S,k-1) + p(S,k-2) + p(S-c,k-1) + 2p(S-c,k-2) \\
&\quad + p(S-d,k-1) + 2p(S-d,k-2) + p(S-c-d,k-2) \\
&\quad + p(S-c-d,k-3) = (1,3,1,0,\cdots,0,0,1,2,0,\cdots,0,0,1,2,0,\cdots, \\
&\quad 0,0,0,1,1,0,\cdots,0)\cdot p_{cd}(S,k), \\
p(G-a,k) &= p(G-a-gd-cf,k) + p(G-a-gd-c-f,k-1) \\
&\quad + p(G-a-g-d-cf,k-1) + p(G-a-g-d-c-f,k-2) \\
&= p(S\cup P_1\cup P_2,k) + p((S-c)\cup P_2,k-1) + p((S-d)\cup P_1\cup P_1,k-1) \\
&\quad + p((S-c-d)\cup P_1,k-2) = p(S,k) + p(S,k-1) + p(S-c,k-1) \\
&\quad + p(S-c,k-2) + p(S-d,k-1) + p(S-c-d,k-2) \\
&= (1,1,0,0,\cdots,0,0,1,1,0,\cdots,0,0,1,0,0,\cdots,0,0,0,1,0,0, \\
&\quad \cdots,0)\cdot p_{cd}(S,k), \\
p(G-b,k) &= p(G-b-gd-cf,k) + p(G-b-gd-c-f,k-1) \\
&\quad + p(G-b-g-d-cf,k-1) + p(G-b-g-d-c-f,k-2) \\
&= p(S\cup P_1\cup P_2,k) + p((S-c)\cup P_1\cup P_1,k-1) + p((S-d)\cup P_2,k-1) \\
&\quad + p((S-c-d)\cup P_1,k-2) = p(S,k) + p(S,k-1) + p(S-c,k-1) \\
&\quad + p(S-d,k-1) + p(S-d,k-2) + p(S-c-d,k-2)
\end{aligned}
$$

$$
\begin{aligned}
&= (1,1,0,0,\cdots,0,0,1,0,0,\cdots,0,0,1,1,0,\cdots,0,0,0,1,0,0,\\
&\cdots,0)\cdot p_{cd}(S,k),\\
p(G-a-b,k) &= p(G-a-b-gd-cf,k)+p(G-a-b-gd-c-f,k-1)\\
&+p(G-a-b-g-d-cf,k-1)+p(G-a-b-g-d-c-f,k-2)\\
&= p(S\cup P_1\cup P_1,k)+p((S-c)\cup P_1,k-1)\\
&+p((S-d)\cup P_1,k-1)+p(S-c-d,k-2)\\
&= p(S,k)+p(S-c,k-1)+p(S-d,k-1)+p(S-c-d,k-2)\\
&= (1,0,0,0,\cdots,0,0,1,0,0,\cdots,0,0,1,0,0,\cdots,0,0,0,1,0,0,\\
&\cdots,0)\cdot p_{cd}(S,k).
\end{aligned}
$$

By the definition of a k-matching vector of G at the edge ab, the vectors

$$(1,3,1,0,\cdots,0,0,1,2,0,\cdots,0,0,1,2,0,\cdots,0,0,0,1,1,0,\cdots,0),$$

$$(1,1,0,0,\cdots,0,0,1,1,0,\cdots,0,0,1,0,0,\cdots,0,0,0,1,0,0,\cdots,0),$$

$$(1,1,0,0,\cdots,0,0,1,0,0,\cdots,0,0,1,1,0,\cdots,0,0,0,1,0,0,\cdots,0)$$

and

$$(1,0,0,0,\cdots,0,0,1,0,0,\cdots,0,0,1,0,0,\cdots,0,0,0,1,0,0,\cdots,0)$$

are the first, $(k+2)$-th, $(2k+3)$-th and $(3k+4)$-th rows of the coefficient matrix, respectively. Moreover, it is need to compute $p(G,k-1),\cdots,p(G,1),p(G,0)$, $p(G-a,k-1),\cdots,$ $p(G-a,1),p(G-a,0)$, $p(G-b,k-1),\cdots,p(G-b,1),p(G-b,0)$ and $p(G-a-b,k-1),\cdots,p(G-a-b,1),p(G-a-b,0)$ to get $p_{ab}(G,k)$. However, there is no need to compute these values separately as we can deduce these values as a product of a vector and $p_{cd}(S,k)$ from the equations above. Thus, after computing the first, $(k+2)$-th, $(2k+3)$-th and $(3k+4)$-th rows, we get the coefficient matrix in the echelon form in every sixteen part, briefly submatrices shown in matrix Q with dashed lines. Consequently, we get $p_{ab}(G,k) = Q\cdot p_{cd}(S,k)$ where the transfer matrix Q is a $4(k+1)\times 4(k+1)$ dimensional matrix. ■

It is clear that when S is isomorphic to P_2 where P_2 is path graph with two vertices, we have

$$p_{ab}(G,k) = Q\cdot\begin{bmatrix} 0 & \cdots & 0 & 1 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 1 \end{bmatrix}^T$$

by the previous theorem.

Theorem 2.2. *Let $G = (V, E)$ be a graph derived from the edge-coalescence of the graph S and a hexagon at the edge fc of S (See Fig. 2). Then*

$$p_{ab}(G, k) = P \cdot p_{fc}(S, k)$$

where the transfer matrix P is a $4(k+1) \times 4(k+1)$ dimensional matrix as follows:

$$\left(\begin{array}{cccccc|cccccc|cccccc|ccccccc}
1 & 3 & 1 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 0 & \cdots & 0 \\
0 & 1 & 3 & 1 & \cdots & 0 & 0 & 0 & 1 & 2 & \cdots & 0 & 0 & 0 & 1 & 2 & \cdots & 0 & 0 & 0 & 0 & 1 & 1 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 3 & 1 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & 0 & \cdots & 0 & 1 & 2 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\
0 & \cdots & 0 & 0 & 1 & 3 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\hline
1 & 2 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 2 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 2 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\hline
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\
0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\hline
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0
\end{array}\right).$$

Proof. It is needed to compute the values $p(G, k), p(G-a, k), p(G-b, k)$ and $p(G-a-b, k)$ by deleting appropriate forms of the edges dc and fa to get the subgraph S apart from the hexagon. Later on, we use the recurrence relations 1 and 2 that are given at the beginning of the section as follows:

$$\begin{aligned}
p(G, k) &= p(G - dc - fa, k) + p(G - dc - f - a, k-1) + p(G - d - c - fa, k-1) \\
&\quad + p(G - d - c - f - a, k-2) = p(S \cup P_4, k) + p((S - f) \cup P_3, k-1) \\
&\quad + p((S - c) \cup P_3, k-1) + p((S - f - c) \cup P_2, k-2) \\
&= p(S, k) + 3p(S, k-1) + p(S, k-2) + p(S - f, k-1) + 2p(S - f, k-2) \\
&\quad + p(S - c, k-1) + 2p(S - c, k-2) + p(S - f - c, k-2) \\
&\quad + p(S - f - c, k-3) = (1, 3, 1, 0, \cdots, 0, 0, 1, 2, 0, \cdots, 0, 0, 1, 2, 0, \cdots, \\
&\quad 0, 0, 0, 1, 1, 0, \cdots, 0) \cdot p_{fc}(S, k), \\
p(G - a, k) &= p(G - a - dc, k) + p(G - a - d - c, k-1) = p(S \cup P_3, k) \\
&\quad + p((S - c) \cup P_2, k-1) = p(S, k) + 2p(S, k-1) + p(S - c, k-1) \\
&\quad + p(S - c, k-2) = (1, 2, 0, 0, \cdots, 0, 0, 0, 0, 0, \cdots, 0, 0, 1, 1, 0, \cdots,
\end{aligned}$$

$$
\begin{aligned}
&0,0,0,0,0,0,\cdots,0)\cdot p_{fc}(S,k),\\
p(G-b,k) &= p(G-b-dc-fa,k)+p(G-b-dc-f-a,k-1)\\
&+p(G-b-d-c-fa,k-1)+p(G-b-d-c-f-a,k-2)\\
&= p(S\cup P_1\cup P_2,k)+p((S-f)\cup P_2,k-1)+p((S-c)\cup P_1\cup P_1,k-1)\\
&+p((S-f-c)\cup P_1,k-2)=p(S,k)+p(S,k-1)+p(S-f,k-1)\\
&+p(S-f,k-2)+p(S-c,k-1)+p(S-f-c,k-2)\\
&=(1,1,0,0,\cdots,0,0,1,1,0,\cdots,0,0,1,0,0,\cdots,\\
&0,0,0,1,0,0,\cdots,0)\cdot p_{fc}(S,k),\\
p(G-a-b,k) &= p(G-a-b-dc,k)+p(G-a-b-d-c,k-1)\\
&= p(S\cup P_2,k)+p((S-c)\cup P_1,k-1)=p(S,k)+p(S,k-1)\\
&+p(S-c,k-1)=(1,1,0,0,\cdots,0,0,0,0,0,\cdots,0,0,1,0,0,\cdots,\\
&0,0,0,0,0,0,\cdots,0)\cdot p_{fc}(S,k).
\end{aligned}
$$

By the definition of a k-matching vector of G at the edge ab, the vectors

$$(1,3,1,0,\cdots,0,0,1,2,0,\cdots,0,0,1,2,0,\cdots,0,0,0,1,1,0,\cdots,0),$$

$$(1,2,0,0,\cdots,0,0,0,0,0,\cdots,0,0,1,1,0,\cdots,0,0,0,0,0,0,\cdots,0),$$

$$(1,1,0,0,\cdots,0,0,1,1,0,\cdots,0,0,1,0,0,\cdots,0,0,0,1,0,0,\cdots,0)$$

and

$$(1,1,0,0,\cdots,0,0,0,0,0,\cdots,0,0,1,0,0,\cdots,0,0,0,0,0,0,\cdots,0)$$

are the first, $(k+2)$-th, $(2k+3)$-th and $(3k+4)$-th rows of coefficient matrix, respectively. Also we need to calculate $p(G,k-1),\cdots,p(G,1),p(G,0)$, $p(G-a,k-1),\cdots$, $p(G-a,1),p(G-a,0)$, $p(G-b,k-1),\cdots,p(G-b,1),p(G-b,0)$, and $p(G-a-b,k-1),\cdots,p(G-a-b,1),p(G-a-b,0)$ to find $p_{ab}(G,k)$. Then, we deduce these values as a product of a vector and $p_{fc}(S,k)$ by using achieved equations above. Then, we have that the coefficient matrix is in the echelon form in every sixteen parts, shortly submatrices shown in matrix P with dashed lines. Consequently, we obtain the equation $p_{ab}(G,k)=P\cdot p_{fc}(S,k)$ where the transfer matrix P is a $4(k+1)\times 4(k+1)$ dimensional matrix. ■

Theorem 2.3. *Let $G=(V,E)$ be a graph derived from the edge-coalescence of the graph S and a hexagon at the edge cd of S (See Fig. 1). Then*

$$p_{bg}(G,k)=R\cdot p_{cd}(S,k)$$

where the transfer matrix R is a $4(k+1)\times 4(k+1)$ dimensional matrix as follows:

$$\left(\begin{array}{cccccc:cccccc:cccccc:ccccccc}
1 & 3 & 1 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 0 & \cdots & 0 \\
0 & 1 & 3 & 1 & \cdots & 0 & 0 & 0 & 1 & 2 & \cdots & 0 & 0 & 0 & 1 & 2 & \cdots & 0 & 0 & 0 & 0 & 1 & 1 & \cdots & 0 \\
\multicolumn{25}{c}{\vdots} \\
0 & \cdots & 0 & 1 & 3 & 1 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & 0 & \cdots & 0 & 1 & 2 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\
0 & \cdots & 0 & 0 & 1 & 3 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\hdashline
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\
\multicolumn{25}{c}{\vdots} \\
0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\
0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\hdashline
1 & 2 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 2 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
\multicolumn{25}{c}{\vdots} \\
0 & \cdots & 0 & 1 & 2 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
\hdashline
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
\multicolumn{25}{c}{\vdots} \\
0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0
\end{array}\right).$$

Proof. As a beginning, by the proof of Theorem 2.1, we have already known the two equation below:

$p(G,k) = (1,3,1,0,\cdots,0,0,1,2,0,\cdots,0,0,1,2,0,\cdots,0,0,0,1,1,0,\cdots,0)\cdot p_{cd}(S,k)$,

$p(G-b,k) = (1,1,0,0,\cdots,0,0,1,0,0,\cdots,0,0,1,1,0,\cdots,0,0,0,1,0,0,\cdots,0)\cdot p_{cd}(S,k)$.

Then, we need to compute just k-matching numbers of the graphs $G-g$ and $G-b-g$ by deleting the edge cf. After that, we use the recurrence relations 1 and 2 as shown below:

$$\begin{aligned}
p(G-g,k) &= p(G-g-cf,k) + p(G-g-c-f,k-1) = p(S\cup P_3,k) \\
&\quad + p((S-c)\cup P_2,k-1) = p(S,k) + 2p(S,k-1) + p(S-c,k-1) \\
&\quad + p(S-c,k-2) = (1,2,0,0,\cdots,0,0,1,1,0,\cdots,0,0,0,0,0,\cdots, \\
&\quad 0,0,0,0,0,0,\cdots,0)\cdot p_{cd}(S,k), \\
p(G-b-g,k) &= p(G-b-g-cf,k) + p(G-b-g-c-f,k-1) \\
&= p(S\cup P_2,k) + p((S-c)\cup P_1,k-1) \\
&= p(S,k) + p(S,k-1) + p(S-c,k-1) \\
&= (1,1,0,0,\cdots,0,0,1,0,0,\cdots,0,0,0,0,0,\cdots,0,0,0,0,0,0,\cdots,0)\cdot p_{cd}(S,k).
\end{aligned}$$

By the definition of a k-matching vector of G at the edge bg, the vectors

$$(1,3,1,0,\cdots,0,0,1,2,0,\cdots,0,0,1,2,0,\cdots,0,0,0,1,1,0,\cdots,0),$$

$$(1,1,0,0,\cdots,0,0,1,0,0,\cdots,0,0,1,1,0,\cdots,0,0,0,1,0,0,\cdots,0),$$

$$(1,2,0,0,\cdots,0,0,1,1,0,\cdots,0,0,0,0,0,\cdots,0,0,0,0,0,0,\cdots,0)$$

and

$$(1,1,0,0,\cdots,0,0,1,0,0,\cdots,0,0,0,0,0,\cdots,0,0,0,0,0,0,\cdots,0)$$

are the first, $(k+2)$-th, $(2k+3)$-th and $(3k+4)$-th rows of coefficient matrix, respectively. Also we need to calculate $p(G,k-1),\cdots,p(G,1),p(G,0)$, $p(G-b,k-1),\cdots,p(G-b,1),p(G-b,0)$, $p(G-g,k-1),\cdots,p(G-g,1),p(G-g,0)$ and $p(G-b-g,k-1),\cdots,p(G-b-g,1),p(G-b-g,0)$ to find $p_{bg}(G,k)$. We derive these values as a product of a vector and $p_{cd}(S,k)$ by using the obtained equations above. Thus, after calculating the first, $(k+2)$-th, $(2k+3)$-th and $(3k+4)$-th rows, we achieve that the coefficient matrix is in the echelon form in every sixteen parts, namely submatrices shown in matrix R with dashed lines. As a result, we get $p_{bg}(G,k) = R \cdot p_{cd}(S,k)$ where the transfer matrix R is a $4(k+1)\times 4(k+1)$ dimensional coefficient matrix. ■

3 Algorithms

In this section, we present two algorithms designed in MATLAB to obtain required transfer matrix forms Q, P, R and $p_{ab}(P_2,k)$ that are introduced in Section 2 more directly. In the first algorithm, based on entered k value, sixteen parts of matrices are obtained in the echelon form that are explained in the proofs of Thms. 2.1, 2.2 and 2.3. In the second algorithm, based on entered k value, for a path graph P_2 with the edge $e = ab$, k-matching vector of P_2 at the edge ab is obtained follows:

$$p_{ab}(P_2,k) = \begin{bmatrix} 0 & \cdots & 0 & 1 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 1 \end{bmatrix}^T.$$

Thanks to the Algorithm 1, we get the transfer matrices Q, P, R for corresponding value of k by adding a few number of steps at the beginning before the step $L(1,:) = L1$. Let us present these steps.

For the transfer matrix Q, it is needed to add the steps consecutively as follows: $L1 = zeros(1, 4*k+4)$; $L1(1) = 1$; $L1(2) = 3$; $L1(3) = 1$; $L1(k+3) = 1$; $L1(k+4) = 2$; $L1(2*k+4) = 1$; $L1(2*k+5) = 2$; $L1(3*k+6) = 1$; $L1(3*k+7) = 1$; $L2 = zeros(1, 4*k+4)$; $L2(1) = 1$; $L2(2) = 1$; $L2(k+3) = 1$; $L2(k+4) = 1$; $L2(2*k+4) = 1$; $L2(3*k+6) = 1$; $L3 = zeros(1, 4*k+4)$; $L3(1) = 1$; $L3(2) = 1$; $L3(k+3) = 1$; $L3(2*k+4) = 1$;

Algorithm 1: Algorithm to set the transfer matrix forms Q, P, R for corresponding k.

Input: Enter the value of k.
Result: Required echelon matrix form according to the rows $1, k+2, 2k+3$ and $3k+4$.

```
L = zeros(4 * k + 4, 4 * k + 4);
"Here, the steps given after this algorithm, will be added according to the desired
  matrix";
L(1, :) = L1;
L(k + 2, :) = L2;
L(2 * k + 3, :) = L3;
L(3 * k + 4, :) = L4;
for from i = 1 to k + 1 do
    for from j = i to k do
        L(i + 1, j + 1) = L(i, j);
        L(i + 1, j + k + 2) = L(i, j + k + 1);
        L(i + 1, j + 2 * k + 3) = L(i, j + 2 * k + 2);
        L(i + 1, j + 3 * k + 4) = L(i, j + 3 * k + 3);
    end
end
for from i = k + 2 to 2 * k + 1 do
    for from j = 1 to k do
        L(i + 1, j + 1) = L(i, j);
        L(i + 1, j + k + 2) = L(i, j + k + 1);
        L(i + 1, j + 2 * k + 3) = L(i, j + 2 * k + 2);
        L(i + 1, j + 3 * k + 4) = L(i, j + 3 * k + 3);
    end
end
for from i = 2 * k + 3 to 3 * k + 2 do
    for from j = 1 to k do
        L(i + 1, j + 1) = L(i, j);
        L(i + 1, j + k + 2) = L(i, j + k + 1);
        L(i + 1, j + 2 * k + 3) = L(i, j + 2 * k + 2);
        L(i + 1, j + 3 * k + 4) = L(i, j + 3 * k + 3);
    end
end
for from i = 3 * k + 4 to 4 * k + 3 do
    for from j = 1 to k do
        L(i + 1, j + 1) = L(i, j);
        L(i + 1, j + k + 2) = L(i, j + k + 1);
        L(i + 1, j + 2 * k + 3) = L(i, j + 2 * k + 2);
        L(i + 1, j + 3 * k + 4) = L(i, j + 3 * k + 3);
    end
end
```

$L3(2*k+5)=1$; $L3(3*k+6)=1$; $L4=zeros(1,4*k+4)$; $L4(1)=1$; $L4(k+3)=1$; $L4(2*k+4)=1$; $L4(3*k+6)=1$;

For the transfer matrix P, it is needed to add the steps consequtively as follows: $L1=zeros(1,4*k+4)$; $L1(1)=1$; $L1(2)=3$; $L1(3)=1$; $L1(k+3)=1$; $L1(k+4)=2$; $L1(2*k+4)=1$; $L1(2*k+5)=2$; $L1(3*k+6)=1$; $L1(3*k+7)=1$; $L2=zeros(1,4*k+4)$; $L2(1)=1$; $L2(2)=2$; $L2(2*k+4)=1$; $L2(2*k+5)=1$; $L3=zeros(1,4*k+4)$; $L3(1)=1$; $L3(2)=1$; $L3(k+3)=1$; $L3(k+4)=1$; $L3(2*k+4)=1$; $L3(3*k+6)=1$; $L4=zeros(1,4*k+4)$; $L4(1)=1$; $L4(2)=1$; $L4(2*k+4)=1$;

For the transfer matrix R, it is needed to add the steps consequtively as follows: $L1=zeros(1,4*k+4)$; $L1(1)=1$; $L1(2)=3$; $L1(3)=1$; $L1(k+3)=1$; $L1(k+4)=2$; $L1(2*k+4)=1$; $L1(2*k+5)=2$; $L1(3*k+6)=1$; $L1(3*k+7)=1$; $L2=zeros(1,4*k+4)$; $L2(1)=1$; $L2(2)=1$; $L2(k+3)=1$; $L2(2*k+4)=1$; $L2(2*k+5)=1$; $L2(3*k+6)=1$; $L3=zeros(1,4*k+4)$; $L3(1)=1$; $L3(2)=2$; $L3(k+3)=1$; $L3(k+4)=1$; $L4=zeros(1,4*k+4)$; $L4(1)=1$; $L4(2)=1$; $L4(k+3)=1$;

Algorithm 2: Algorithm to set $p_{ab}(P_2,k)$, where a and b are vertices of P_2.

Input: Enter the value of k.
Result: $p_{ab}(P_2,k)$.
$M=zeros(1,4*k+4)$;
$M(k)=1$;
$M(k+1)=1$;
$M(2*k+2)=1$;
$M(3*k+3)=1$;
$M(4*k+4)=1$;
$V=transpose(M)$;

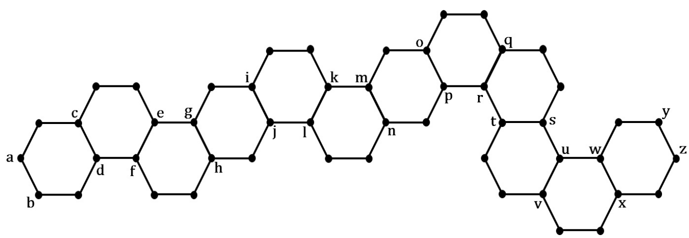

Figure 3. A benzenoid chain used in Example 3.1

Example 3.1. *Let G be a benzenoid chain as shown in Fig. 3. Then let us calculate the 25-matching number $p(G,25)$ of G by using the vector $p_{ab}(G,25)$ and Thms. 2.1, 2.2, 2.3:*

$p_{ab}(G,25) \quad = \quad Q \cdot R \cdot P \cdot Q \cdot R \cdot P \cdot Q \cdot R \cdot R \cdot P \cdot P \cdot Q \cdot p_{yz}(P_2,25).$

Then by using two algorithms (in MATLAB) to get Q, P, R *and* $p_{yz}(P_2,25)$ *the result is achieved as follows:*

$p_{ab}(G,25)$	$=[295$	26797	852250	13424314	123419183
730990381	2978491338	8744585185	19135395999	32010001312	41726187514
43004516257	35425168253	23506162672	12627874147	5506347162	1948864426
558326651	128704829	23635365	3404687	375772	30634
1736	61	1	$\cdots$	58	$1]^T$.

As a result, we get $p(G,25) = 295, p(G,24) = 26797, p(G,23) = 852250, \cdots,$ $p(G,3) = 30634,$ $p(G,2) = 1736, p(G,1) = 61$ *and* $p(G,0) = 1.$

As shown in the example, every k-matching number can be calculated by utilizing the defined k-matching vector and the transfer matrices Q, P, R that are obtained in Thms. 2.1, 2.2, 2.3 for any benzenoid chain. Moreover, thanks to k-matching vector and Thms.2.1, 2.2, 2.3, not only k-matching numbers of any benzenoid chain but also Hosoya index of the corresponding benzenoid chain can be achieved.

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