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Enumerating *k*-Matchings in Cyclic Chains Using the Transfer Matrix Technique

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Abstract

A cyclic chain is a plane graph whose all inner faces are cycles and its inner dual is isomorphic to a path. In this paper, the transfer matrix technique using the k-matching vector is developed to compute the number of k-matchings in an arbitrary cyclic chain. This extends similar methods developed earlier in two papers for benzenoid chains and for octagonal chains. The method is illustrated on the flourene molecule.

1 Introduction

Matchings play an important role in chemical graph theory. This is in particular evident from the fact that perfect matchings are chemically termed Kekulé structures. More precisely, these structures are diagrams for hydrocarbon molecules that identify the location of single and double carbon bonds. The location of these double bonds thus corresponds to a perfect matching for a graph, cf. [2]. For the theory on the Kekulé structures in benzenoid hydrocarbons we recommend the book [4].

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The number of perfect matchings in a molecular graph describes the extent of its aromatic property and is also used in the analysis of resonance energy and stability of certain chemical compounds, cf. [8]. Now, the Hosoya index [7] of a (molecular) graph is the total number of its matchings. Since its introduction, the index has received a great deal of attention. As a starting point, we suggest the recent papers [5, 10], references therein, and the survey paper [17].

The transfer matrix technique goes back to [14, 15], where it was designed to investigate the matching polynomial, the Hosoya index, the characteristic polynomial, and the Wiener index of benzenoid chains. The essence of the technique is to assign a vector v to the corresponding benzenoid system and then, by multiplying v with an appropriate transfer matrix, obtain the desired invariant for the benzenoid system with one more hexagon. In [3], Cruz, Marín and Rada followed by introducing the Hosoya vector to apply the transfer matrix technique to the Hosoya index of catacondensed hexagonal systems.

In [12], Oz and Cangul modified the transfer matrix technique by introducing the k-matching vector to compute the number of k-matchings in an arbitrary benzenoid chain; summing over all k we of course get the Hosoya index of the chain. The method was adopted in [1] to work on chains consisting of 8-cycles. In [11] Oz further extended the method to be applicable on arbitrary catacondensed benzenoid systems, that is, also in the branched case. Using this approach, Shi and Deng [16] proved that the number of maximal matchings of a benzenoid chain with n hexagons equals to the product of n certain matrices, and also obtained the number of perfect matchings of all benzenoid chains. Moreover, in [13] the method was applied to primitive coronoid systems, and in [6] to specific classes of pericondensed benzenoid systems. We also mention that in [9], a method to compute the number of k-matchings in hexagonal systems was presented for $k \leq 5$.

In this paper we demonstrate that the transfer matrix method which uses the k-matching vector can be extended to arbitrary cyclic chains. This generalizes and unifies the method from [12] which works on benzenoid chains and the method from [1] which works on octagonal chains.

In the next section concepts needed are formally introduced, a couple of known results recalled, and the essence of the transfer matrix method explained. In Section 3, the transfer matrix method to compute the k-matching vector of an arbitrary cyclic chain is developed. The transfer matrices corresponding to all possible situations/edges, where the next cycle of the cyclic chain will be attached to the present cyclic chain, are derived in three theorems. In the final section the method developed is illustrated on a chemical graph corresponding to the fluorene molecule.

2 Preliminaries

Let $G = (V(G), E(G))$ be a graph. A *matching* of G is a set of edges $M \subseteq E(G)$ such that no two edges from M share a vertex. If $|M| = k$, then M is a *k-matching.* The *Hosoya index* $Z(G)$ of G is the total number of different matchings of G. Denoting by $p(G,k)$ the number of k-matchings of G we have $Z(G) = \sum_{k\geq 0} p(G,k)$. A *cyclic chain* is a plane graph whose all inner faces are cycles and its inner dual is isomorphic to a path. For examples of cyclic chains together with their inner duals see Fig. 1.

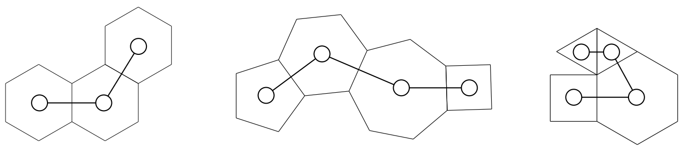

Figure 1. Examples of cyclic chains and their inner duals (paths).

We next recall two straightforward, but utmost useful lemmas.

Lemma 1. *If ab is an edge of a graph G, then*

$$p(G,k) = p(G - ab, k) + p(G - a - b, k - 1)\,.$$

Lemma 2. *If G is a graph consisting of two components G_1 and G_2, then*

$$p(G,k) = p(G_1 \cup G_2, k) = \sum_{i=0}^{k} p(G_1, i) p(G_2, k-i)\,.$$

To conclude the preliminaries we briefly describe the transfer matrix method applied to cyclic chains. The key concept of the method is the following vector. If ab is an edge of a graph G, then the *k-matching vector* $p_{ab}(G,k)$ of G with respect to ab is the vector

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

Let now G be a cyclic chain consisting of t consecutive cycles $C^{(i)}$, $i \in [t]$, and let $u'v'$ be the edge shared by $C^{(t-1)}$ and $C^{(t)}$. Let further G' be the cyclic chain consisting of the $t-1$ cycles $C^{(i)}$, $i \in [t-1]$. Then we aim to find a matrix X, called a *transfer matrix*, such that $p_{uv}(G,k) = X \cdot p_{u'v'}(G',k)$. Here the edge uv of $C^{(t)}$ is conceived as the edge to which we will attach a new cycle to extend G to a cyclic chain consisting of $t+1$ cycles.

3 Determining the transfer matrices

As said, our goal is to use the transfer matrix method to compute the k-matching vector of an arbitrary cyclic chain. For this sake, we need to determine the transfer matrices corresponding to all possible situations/edges, where the next cycle of the cyclic chain will be attached to the present cyclic chain. All possible cases are collected in three theorems, where we will denote the consecutive vertices of an attached cycle as $a_1, a_2, \ldots, a_n$. In all the cases we are going to determine $p_{a_1 a_n}(G, k)$, that is, the edge $a_1 a_n$ is considered at the edge at which the next cycle of the cyclic chain will be attached.

To describe the transfer matrices that will occur in a reasonable way, the following auxiliary matrices are useful. For a predefined positive integer k, we define $M(G)$, $0M(G)$, and $00M(G)$ as the upper triangular Toeplitz matrices of dimension $(k+1) \times (k+1)$, whose first rows are respectively as follows:

$$[p(G,0), p(G,1), p(G,2), \ldots, p(G,k)]\,,$$
$$[0, p(G,0), p(G,1), p(G,2), \ldots, p(G,k-1)]\,,$$
$$[0, 0, p(G,0), p(G,1), p(G,2), \ldots, p(G,k-2)]\,.$$

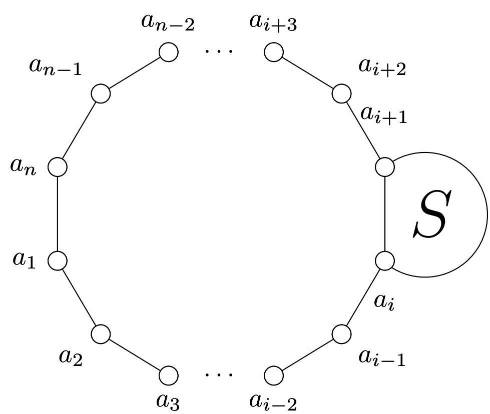

Figure 2. Graph used in Theorem 1.

Theorem 1. *Let S be a graph, and let G be obtained from the disjoint union of S and C_n by identifying the edge $a_i a_{i+1}$, $i \in \{2, 3, \ldots, n-2\}$ of C_n, with an edge of G, see Fig. 2. Then*

$$p_{a_1 a_n}(G, k) = A_{n_i} \cdot p_{a_i a_{i+1}}(S, k)\,,$$

where A_{n_i} is the $4(k+1) \times 4(k+1)$ matrix with the block structure as shown in Fig. 3.

$$\begin{array}{c|c|c|c}
M(P_{n-2}) & 0M(P_{n-3}) & 0M(P_{n-3}) & 00M(P_{n-4}) \\
\hline
M(P_{i-2} \cup P_{n-i-1}) & 0M(P_{i-3} \cup P_{n-i-1}) & 0M(P_{i-2} \cup P_{n-i-2}) & 00M(P_{i-3} \cup P_{n-i-2}) \\
\hline
M(P_{i-1} \cup P_{n-i-2}) & 0M(P_{i-2} \cup P_{n-i-2}) & 0M(P_{i-1} \cup P_{n-i-3}) & 00M(P_{i-2} \cup P_{n-i-3}) \\
\hline
M(P_{i-2} \cup P_{n-i-2}) & 0M(P_{i-3} \cup P_{n-i-2}) & 0M(P_{i-2} \cup P_{n-i-3}) & 00M(P_{i-3} \cup P_{n-i-3})
\end{array}$$

Figure 3. Matrix A_{n_i}.

Proof. To begin consider the $p(G, k)$, first component of $p_{a_1 a_2}(G, k)$. Setting $X = p(G, k)$ and applying Lemmas 1 and 2 we can compute in the following way:

$$\begin{aligned}
X &= p(G - a_{i-1}a_i - a_{i+1}a_{i+2}, k) \\
&\quad + p(G - a_{i-1} - a_i - a_{i+1}a_{i+2}, k-1) \\
&\quad + p(G - a_{i-1}a_i - a_{i+1} - a_{i+2}, k-1) \\
&\quad + p(G - a_{i-1} - a_i - a_{i+1} - a_{i+2}, k-2) \\
&= p(S \cup P_{n-2}, k) + p((S - a_i) \cup P_{n-3}, k-1) \\
&\quad + p((S - a_{i+1}) \cup P_{n-3}, k-1) \\
&\quad + p(S - a_i - a_{i+1} \cup P_{n-4}, k-2) \\
&= \Big(p(P_{n-2}, 0), p(P_{n-2}, 1), p(P_{n-2}, 2), \ldots, p(P_{n-2}, k), \\
&\quad 0, p(P_{n-3}, 0), p(P_{n-3}, 1), \ldots, p(P_{n-3}, k-1), \\
&\quad 0, p(P_{n-3}, 0), p(P_{n-3}, 1), \ldots, p(P_{n-3}, k-1), \\
&\quad 0, 0, p(P_{n-4}, 0), \ldots, p(P_{n-4}, k-2)\Big) p_{a_i a_{i+1}}(S, k)\,.
\end{aligned}$$

The obtained vector corresponds to the first row of the matrix A_{n_i}.

The above proof similarly holds for the second component of the vector $p_{a_1a_2}(G,k)$, therefore we can state:

$$\begin{aligned}p(G,k-1) = \Big(&0, p(P_{n-2},0), p(P_{n-2},1), \dots, p(P_{n-2},k-1),\\ &0,0,p(P_{n-3},0), p(P_{n-3},1), \dots, p(P_{n-3},k-2),\\ &0,0,p(P_{n-3},0), p(P_{n-3},1), \dots, p(P_{n-3},k-2),\\ &0,0,0,p(P_{n-4},0), \dots, p(P_{n-4},k-3)\Big)p_{a_ia_{i+1}}(S,k)\,.\end{aligned}$$

In a similar manner, we obtain the remaining $k-1$ components of the form $p(G,i)$, where $0 \le i < k-1$. Thus, we have obtained four upper triangular Toeplitz matrices of dimension $(k+1)\times(k+1)$ which lie above in the matrix A_{n_i}.

Analogous to the calculation of $p(G,k)$, setting $X_1 = p(G-a_1,k)$, $X_n = p(G-a_n,k)$, and $X_{1n} = p(G-a_1-a_n,k)$, we proceed to compute X_1, X_n, and X_{1n} as follows.

$$\begin{aligned}X_1 &= p(G-a_1-a_{i-1}a_i-a_{i+1}a_{i+2},k)\\ &\quad + p(G-a_1-a_{i-1}-a_i-a_{i+1}a_{i+2},k-1)\\ &\quad + p(G-a_1-a_{i-1}a_i-a_{i+1}-a_{i+2},k-1)\\ &\quad + p(G-a_1-a_{i-1}-a_i-a_{i+1}-a_{i+2},k-2)\\ &= p(S\cup P_{i-2}\cup P_{n-i-1},k)\\ &\quad + p((S-a_i)\cup P_{i-3}\cup P_{n-i-1},k-1)\\ &\quad + p((S-a_{i+1})\cup P_{i-2}\cup P_{n-i-2},k-1)\\ &\quad + p(S-a_i-a_{i+1}\cup P_{i-3}\cup P_{n-i-2},k-2)\\ &= \Big(p(P_{i-2}\cup P_{n-i-1},0), p(P_{i-2}\cup P_{n-i-1},1), \dots, p(P_{i-2}\cup P_{n-i-1},k),\\ &\quad 0, p(P_{i-3}\cup P_{n-i-1},0), \dots, p(P_{i-3}\cup P_{n-i-1},k-1),\\ &\quad 0, p(P_{i-2}\cup P_{n-i-2},0), \dots, p(P_{i-2}\cup P_{n-i-2},k-1),\\ &\quad 0,0,p(P_{i-3}\cup P_{n-i-2},0), \dots, p(P_{i-3}\cup P_{n-i-2},k-2)\Big)\cdot p_{a_ia_{i+1}}(S,k)\,.\end{aligned}$$

$$\begin{aligned}X_n = \Big(&p(P_{i-1}\cup P_{n-i-2},0), p(P_{i-1}\cup P_{n-i-2},1), \dots, p(P_{i-1}\cup P_{n-i-2},k),\\ &0, p(P_{i-2}\cup P_{n-i-2},0), \dots, p(P_{i-2}\cup P_{n-i-2},k-1),\\ &0, p(P_{i-1}\cup P_{n-i-3},0), \dots, p(P_{i-1}\cup P_{n-i-3},k-1),\end{aligned}$$

$$0, 0, p(P_{i-2} \cup P_{n-i-3}, 0), \dots, p(P_{i-2} \cup P_{n-i-3}, k-2)\Big) \cdot p_{a_i a_{i+1}}(S, k)\,.$$

$$\begin{aligned} X_{1n} = \Big(&p(P_{i-2} \cup P_{n-i-2}, 0), p(P_{i-2} \cup P_{n-i-2}, 1), \dots, p(P_{i-2} \cup P_{n-i-2}, k),\\ &0, p(P_{i-3} \cup P_{n-i-2}, 0), \dots, p(P_{i-3} \cup P_{n-i-2}, k-1),\\ &0, p(P_{i-2} \cup P_{n-i-3}, 0), \dots, p(P_{i-2} \cup P_{n-i-3}, k-1),\\ &0, 0, p(P_{i-3} \cup P_{n-i-3}, 0), \dots, p(P_{i-3} \cup P_{n-i-3}, k-2)\Big) \cdot p_{a_i a_{i+1}}(S, k)\,. \end{aligned}$$

The same reasoning applies to the three computed components as it did for the first $k+1$ components. Thus, we obtain the remaining matrices that form the matrix A_{n_i}.

We can conclude that $p_{a_1 a_n}(G, k) = A_{n_i} \cdot p_{a_i a_{i+1}}(S, k)$, where A_{n_i} is the matrix shown in Fig. 3. ∎

We continue with our second main result, which reads as follows.

Theorem 2. *Let S be a graph, and let G be the graph obtained from the disjoint union of S and C_n by identifying the edge $a_1 a_2$ of C_n, with an edge of G. Then*

$$p_{a_1 a_n}(G, k) = A_{n_1} \cdot p_{a_1 a_2}(S, k)\,,$$

where A_{n_1} is the $4(k+1) \times 4(k+1)$ matrix shown in Fig. 4.

$$\left(\begin{array}{c:c:c:c} M(P_{n-2}) & 0M(P_{n-3}) & 0M(P_{n-3}) & 00M(P_{n-4}) \\ \hdashline 0 & M(P_{n-2}) & 0 & 0M(P_{n-3}) \\ \hdashline M(P_{n-3}) & 0 & 0M(P_{n-4}) & 0 \\ \hdashline 0 & M(P_{n-3}) & 0 & 0M(P_{n-4}) \end{array}\right)$$

Figure 4. Matrix A_{n_1}.

Proof. Setting $X = p(G, k)$, $X_1 = p(G - a_1, k)$, $X_n = p(G - a_n, k)$ and $X_{1n} = p(G - a_1 - a_n, k)$, we can compute as follows:

$$X = p(G - a_1 a_n - a_2 a_3, k) + p(G - a_1 - a_n - a_2 a_3, k-1)$$

$$
\begin{aligned}
&+ p(G - a_1 a_n - a_2 - a_3, k-1)\\
&+ p(G - a_n - a_1 - a_2 - a_3, k-2)\\
&= p(S \cup P_{n-2}, k) + p((S - a_1) \cup P_{n-3}, k-1)\\
&+ p((S - a_2) \cup P_{n-3}, k-1)\\
&+ p((S - a_1 - a_2) \cup P_{n-4}, k-2)\\
&= \Big(p(P_{n-2}, 0), p(P_{n-2}, 1), p(P_{n-2}, 2), \ldots, p(P_{n-2}, k),\\
&0, p(P_{n-3}, 0), p(P_{n-3}, 1), \ldots, p(P_{n-3}, k-1),\\
&0, p(P_{n-3}, 0), p(P_{n-3}, 1), \ldots, p(P_{n-3}, k-1),\\
&0, 0, p(P_{n-4}, 0), \ldots, p(P_{n-4}, k-2) \Big) \cdot p_{a_1 a_2}(S, k)\,.
\end{aligned}
$$

$$
\begin{aligned}
X_1 &= p(G - a_1 - a_2 a_3, k) + p(G - a_1 - a_2 - a_3, k-1)\\
&= p((S - a_1) \cup P_{n-2}, k) + p((S - a_1 - a_2) \cup P_{n-3}, k-1)\\
&= \Big(0, \quad 0, \quad 0, \quad \ldots, \quad 0,\\
&\quad p(P_{n-2}, 0), p(P_{n-2}, 1), p(P_{n-2}, 2) \ldots, p(P_{n-2}, k),\\
&\quad 0, \quad 0, \quad 0, \quad \ldots, \quad 0,\\
&\quad 0, p(P_{n-3}, 0), p(P_{n-3}, 1), \ldots, p(P_{n-3}, k-1) \Big) \cdot p_{a_1 a_2}(S, k)\,.
\end{aligned}
$$

$$
\begin{aligned}
X_n &= p(G - a_n - a_2 a_3, k) + p(G - a_n - a_2 - a_3, k-1)\\
&= p(S \cup P_{n-3}, k) + p((S - a_2) \cup P_{n-4}, k-1)\\
&= \Big(p(P_{n-3}, 0), p(P_{n-3}, 1), p(P_{n-3}, 2) \ldots, p(P_{n-3}, k),\\
&\quad 0, \quad 0, \quad 0, \quad \ldots, \quad 0,\\
&\quad 0, p(P_{n-4}, 0), p(P_{n-4}, 1), \ldots, p(P_{n-4}, k-1),\\
&\quad 0, \quad 0, \quad 0, \quad \ldots, \quad 0 \Big) \cdot p_{a_1 a_2}(S, k)\,.
\end{aligned}
$$

$$
\begin{aligned}
X_{1n} = &\Big(0, \quad 0, \quad 0, \quad \ldots, \quad 0,\\
&p(P_{n-3}, 0), p(P_{n-3}, 1), p(P_{n-3}, 2) \ldots, p(P_{n-3}, k),
\end{aligned}
$$

$$0, \quad 0, \quad 0, \quad \ldots, \quad 0,$$
$$0, p(P_{n-4}, 0), p(P_{n-4}, 1), \ldots, p(P_{n-4}, k-1)\Big) \cdot p_{a_1 a_2}(S, k)\,.$$

Therefore, it holds that $p_{a_1 a_n}(G, k) = A_{n_1} \cdot p_{a_1 a_2}(S, k)$, where A_{n_1} is the matrix shown in Fig. 4. ∎

Our final main result is the following.

Theorem 3. *Let S be a graph, and let G be the graph obtained from the disjoint union of S and C_n by identifying the edge $a_{n-1}a_n$ of C_n, with an edge of G. Then*

$$p_{a_1 a_n}(G, k) = A_{n_{n-1}} \cdot p_{a_{n-1} a_n}(S, k)\,,$$

where $A_{n_{n-1}}$ is the $4(k+1) \times 4(k+1)$ matrix shown in Fig. 5.

$$\left(\begin{array}{c:c:c:c}
M(P_{n-2}) & 0M(P_{n-3}) & 0M(P_{n-3}) & 00M(P_{n-4}) \\ \hdashline
M(P_{n-3}) & 0M(P_{n-4}) & 0 & 0 \\ \hdashline
0 & 0 & M(P_{n-2}) & 0M(P_{n-3}) \\ \hdashline
0 & 0 & M(P_{n-3}) & 0M(P_{n-4})
\end{array}\right)$$

Figure 5. Matrix $A_{n_{n-1}}$.

Proof. Setting $X = p(G, k)$, $X_1 = p(G - a_1, k)$, $X_n = p(G - a_n, k)$ and $X_{1n} = p(G - a_1 - a_n, k)$, we can compute as follows:

$$\begin{aligned}
X &= p(G - a_{n-2}a_{n-1} - a_n a_1, k) + p(G - a_{n-2} - a_{n-1} - a_n a_1, k-1) \\
&\quad + p(G - a_{n-2}a_{n-1} - a_n - a_1, k-1) \\
&\quad + p(G - a_{n-2} - a_{n-1} - a_n - a_1, k-2) \\
&= p(S \cup P_{n-2}, k) + p((S - a_{n-1}) \cup P_{n-3}, k-1) \\
&\quad + p((S - a_n) \cup P_{n-3}, k-1)
\end{aligned}$$

$$
\begin{aligned}
&+ p((S - a_{n-1} - a_n) \cup P_{n-4}, k-2) \\
=&\Big(p(P_{n-2},0), p(P_{n-2},1), p(P_{n-2},2), \ldots, p(P_{n-2},k), \\
&0, p(P_{n-3},0), p(P_{n-3},1), \ldots, p(P_{n-3},k-1), \\
&0, p(P_{n-3},0), p(P_{n-3},1), \ldots, p(P_{n-3},k-1), \\
&0, 0, p(P_{n-4},0), \ldots, p(P_{n-4},k-2)\Big) \cdot p_{a_{n-1}a_n}(S,k) \,.
\end{aligned}
$$

$$
\begin{aligned}
X_1 &= p(G - a_1 - a_{n-2}a_{n-1}, k) + p(G - a_1 - a_{n-2} - a_{n-1}, k-1) \\
&= p(S \cup P_{n-3}, k) + p((S - a_{n-1}) \cup P_{n-4}, k-1) \\
&=\Big(p(P_{n-3},0), p(P_{n-3},1), p(P_{n-3},2) \ldots, p(P_{n-3},k), \\
&\quad 0, p(P_{n-4},0), p(P_{n-4},1) \ldots, p(P_{n-4},k-1), \\
&\quad 0, \quad 0, \quad 0, \quad \ldots, \quad 0, \\
&\quad 0, \quad 0, \quad 0, \quad \ldots, \quad 0\Big) \cdot p_{a_{n-1}a_n}(S,k) \,.
\end{aligned}
$$

$$
\begin{aligned}
X_n &= p(G - a_n - a_{n-1}a_{n-2}, k) + p(G - a_n - a_{n-1} - a_{n-2}, k-1) \\
&= p((S - a_n) \cup P_{n-2}, k) + p((S - a_{n-1} - a_n) \cup P_{n-3}, k-1) \\
&=\Big(0, \quad 0, \quad 0, \quad \ldots, \quad 0, \\
&\quad 0, \quad 0, \quad 0, \quad \ldots, \quad 0, \\
&\quad p(P_{n-2},0), p(P_{n-2},1), \ldots, p(P_{n-2},k), \\
&\quad 0, p(P_{n-3},0), \ldots, p(P_{n-3},k-1)\Big) \cdot p_{a_{n-1}a_n}(S,k) \,.
\end{aligned}
$$

$$
\begin{aligned}
X_{1n} =&\Big(0, \quad 0, \quad 0, \quad \ldots, \quad 0, \\
&0, \quad 0, \quad 0, \quad \ldots, \quad 0, \\
&p(P_{n-3},0), p(P_{n-3},1), \ldots, p(P_{n-3},k), \\
&0, p(P_{n-4},0), \ldots, p(P_{n-4},k-1)\Big) \cdot p_{a_{n-1}a_n}(S,k) \,.
\end{aligned}
$$

Therefore, $p_{a_1a_n}(G,k) = A_{n_{n-1}} \cdot p_{a_{n-1}a_n}(S,k)$, where $A_{n_{n-1}}$ is the matrix shown in Fig. 5. ■

Due to the symmetry of the cycles, $A_{n_{n-1}} = R \cdot A_{n_1} \cdot R$, where R is the following $4(k+1) \times 4(k+1)$ dimensional matrix:

$$\begin{pmatrix} I_{k+1} & 0 & 0 & 0 \\ 0 & 0 & I_{k+1} & 0 \\ 0 & I_{k+1} & 0 & 0 \\ 0 & 0 & 0 & I_{k+1} \end{pmatrix}.$$

4 An example

For an example how the method developed in this paper works, consider the graph F of the fluorene molecule, see Fig. 6.

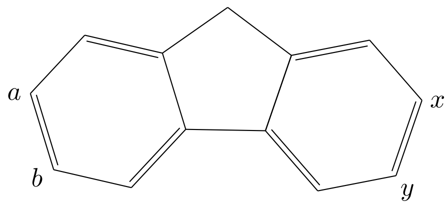

Figure 6. The graph F of fluorene and its maximum matching.

Denoting by $p_{ab}(F,6)|_{k+1}$ the vector $p_{ab}(F,6)$ restricted to its first $k+1$ components, we have:

$$\begin{aligned} p_{ab}(F,6)|_{k+1} &= (A_{6_3} \cdot A_{5_2} \cdot A_{6_3} \cdot p_{xy}(P_2,6))|_{k+1} \\ &= [22, 141, 273, 220, 84, 15, 1]^T , \end{aligned}$$

where the matrix A_{6_3} is the same as the matrix Q in [12], and the matrix A_{5_2} can be computed using Theorem 1 as follows:

$$A_{5_2} = \left(\begin{array}{c:c:c:c} M(P_3) & 0M(P_2) & 0M(P_2) & 00M(P_1) \\ \hdashline M(P_0 \cup P_2) & 0M(P_{-1} \cup P_2) & 0M(P_0 \cup P_1) & 00M(P_{-1} \cup P_1) \\ \hdashline M(P_1 \cup P_1) & 0M(P_0 \cup P_1) & 0M(P_1 \cup P_0) & 00M(P_0 \cup P_0) \\ \hdashline M(P_0 \cup P_1) & 0M(P_{-1} \cup P_1) & 0M(P_0 \cup P_0) & 00M(P_{-1} \cup P_0) \end{array}\right).$$

It is important to note that $p(P_0) = 1$ and that $p(P_{-i}) = 0$ for $i \in \mathbb{N}^+$. Given that the largest graph which appears within the adjacency matrix A_{5_2} is P_3, it suffices to compute just 1-matchings. Therefore, setting the first row of matrices $M(a,b)$, $0M(a,b)$ and $00M(a,b)$ respectively as:

$$[a, b, 0, \ldots, 0], \quad [0, a, b, 0, \ldots, 0], \quad [0, 0, a, b, 0, \ldots, 0],$$

the matrix A_{5_2} can be written as follows:

$$A_{5_2} = \left(\begin{array}{c|c|c|c} M(1,2) & 0M(1,1) & 0M(1,1) & 00M(1,0) \\ \hline M(1,1) & 0 & 0M(1,0) & 0 \\ \hline M(1,0) & 0M(1,0) & 0M(1,0) & 00M(1,0) \\ \hline M(1,0) & 0 & 0M(1,0) & 0 \end{array}\right).$$

Note that since $p_{ab}(F,6)|_{k+1} = [22, 141, 273, 220, 84, 15, 1]^T$, we can conclude that $Z(F) = 22 + 141 + 273 + 220 + 84 + 15 + 1 = 756$.

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