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Some Remarks on the Matching Polynomial and Its Zeros

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The matching polynomial (also called reference and acyclic polynomial) was discovered in chemistry, physics and mathematics at least six times. We demonstrate that the matching polynomial of a bipartite graph coincides with the rook polynomial of a certain board. The basic notions of rook theory[17] are described. It is also shown that the matching polynomial cannot always discriminate between planar isospectral molecules.

INTRODUCTION

Four papers[1-4] which have been recently published in chemical journals consider the question of the reality of the zeros of the matching polynomial. Therefore it might be useful for theoretical chemists to know that similar or even equivalent problems have been examined in mathematics and theoretical physics some time ago.

A k-matching of a graph G is a subgraph of G consisting of k pairs of vertices, each pair being connected by an edge. If $p(G, k)$ denotes the number of k-matchings of a graph G with n vertices, then

$$\alpha(G) = \alpha(G, x) = \sum_k (-1)^k p(G, k) x^{n-2k} \tag{1}$$

is the matching polynomial of G.

Various authors have proposed different names for $\alpha(G)$, namely reference polynomial[1,3,4,5], acyclic polynomial[6,7,8] and matching polynomial[2,4,9,10,11]. This polynomial plays a significant role in statistical physics (theory of monomer-dimer systems) and quantum organic chemistry (theory of aromaticity). For both theories it is rather important that all the roots of the equation $\alpha(G, x) = 0$ be real numbers. It is therefore not surprising that numerous efforts have been made to establish this fact[1-4, 12-15].

Because of the several independent discoveries of $\alpha(G)$, which were usually not noticed by researchers working in other fields of science, it may be useful to give a short review of the history of this problem.

The idea of matching is one of the oldest concepts of graph theory and therefore much work has been done on the numbers $p(G, k)$[16,17]. Another related topic in combinatorics is the theory of permutations with restrictions, where the numbers $r(B, k)$ play a central role[17].

The polynomial

$$R(B) = R(B, x) = \sum_k r(B, k)\, x^k \tag{2}$$

is known[17] as the rook polynomial. Instead of $R(B)$, the associated rook polynomial

$$\varrho(B) = \varrho(B, x) = \sum_k (-1)^k\, r(B, k)\, x^{a+b-2k} \tag{3}$$

is sometimes considered. $\varrho(B)$ is related in an obvious manner to $R(B)$ and has moreover a form similar to $\alpha(G)$, eq. (1). (The meaning of the symbols B, $r(B, k)$, a and b will be explained in the next section).

The theory of rook polynomials was elaborated in combinatorial analysis some thirty years ago[17]. Within this theory it was conjectured[18] and immediately thereafter also proved[19] that all the roots of the equation $\varrho(B, x) = 0$ are real numbers.

For a long time, however, the close connection between $\varrho(B)$ and $\alpha(G)$ was not recognized.

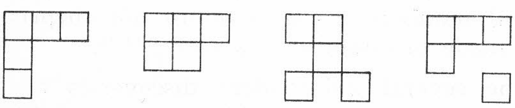
The first contributions to the theory of the matching polynomial came from statistical physics. A result which is equivalent with the statement that all the roots of $\alpha(G, x) = 0$ are real was first communicated by Heilmann and Lieb[12] in 1970 and at the same time independently by Kunz[14]. These authors later developed[13,15] a detailed theory of $\alpha(G)$. Theoretical chemists, unfortunately, seem to have become aware of the papers[12–15] only in the second half of 1978. In the meantime Hosoya[20] used the polynomial

$$Q(G, x) = \sum_k p(G, k)\, x^k \tag{4}$$

in the study of the thermodynamic behaviour of saturated hydrocarbons. Aihara[5] and independently Gutman, Milun and Trinajstić[6] introduced $\alpha(G)$ within a novel theory of aromaticity. (For further references on the chemical applications of $\alpha(G)$ see[10]). Without knowledge of the previous work by Heilmann, Lieb and Kunz, the reality of the zeros of $\alpha(G)$ was first conjectured[7,8] and later proved[2]. Finally, few years ago Farrell considered in a mathematical paper[9], the basic properties of $\alpha(G)$ and thus he discovered $\alpha(G)$ for the sixth time (of course, not being aware of any of the previous publications). Farrell was the first to use the name »matching polynomial«.

THE ROOK THEORY AND ITS CONNECTION WITH THE MATCHING POLYNOMIALS

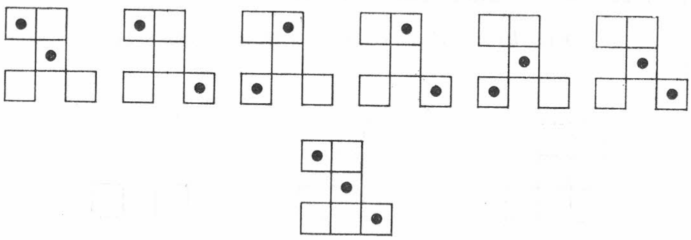
By a board B we mean a subset of cells of an $m \times m$ chessboard. For example, B_1, B_2, B_3 and B_4 are boards.



B_1 B_2 B_3 B_4

The number of rows and columns in B will be denoted by $a = a(B)$ and $b = b(B)$, respectively. Thus, $a(B_1) = a(B_3) = a(B_4) = 3$, $a(B_2) = 2$, $b(B_1) = b(B_2) = b(B_3) = b(B_4) = 3$.

The number of ways in which one can arrange k non-attacking rooks on B is denoted by $r(B, k)$. By definition, $r(B, 0) = 1$ for all boards. As an example we present all the six possible arrangements of two rooks and the unique arrangement of three rooks on the board B_3.



Consequently $r(B_3, 2) = 6$, $r(B_3, 3) = 1$. The rook polynomials of the boards B_1, B_2, B_3 and B_4 can be calculated in this manner. They read

$$R(B_1, x) = 1 + 5x + 4x^2$$
$$R(B_2, x) = 1 + 5x + 4x^2$$
$$R(B_3, x) = 1 + 5x + 6x^2 + x^3$$
$$R(B_4, x) = 1 + 5x + 4x^2 + x^3$$

while the corresponding ϱ-polynomials are

$$\varrho(B_1) = x^6 - 5x^4 + 4x^2$$
$$\varrho(B_2) = x^5 - 5x^3 + 4x$$
$$\varrho(B_3) = x^6 - 5x^4 + 6x^2 - 1$$
$$\varrho(B_4) = x^6 - 5x^4 + 4x^2 - 1$$

Among the numerous known results in the rook theory[17], we shall mention the following.

1. For every board B,

$$r(B, 1) = \text{number of cells in } B$$
$$r(B, k) = 1 \Rightarrow r(B, k+1) = 0$$
$$r(B, k) = 0 \Rightarrow r(B, k+1) = 0$$

2. If the board B is composed of two subboards B_1 and B_2 so that no cell from B_1 lies in a row or column in which there is a cell from B_2, then

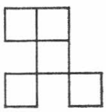
$$R(B) = R(B_1)\, R(B_2); \qquad \varrho(B) = \varrho(B_1)\, \varrho(B_2)$$

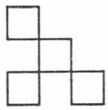
3. Let c_{ij} denotes the cell in the i'th row and j'th column of the board B. Let $B - c_{ij}$ be a board obtained from B by deleting the cell c_{ij}. Let $B - C_{ij}$ be the board obtained by deleting from B the i-th row and the j-th column.

An arrangement of k non-attacking rooks either contains a rook in the cell c_{ij} or not. If there is a rook in c_{ij}, then no other rooks can be placed in the cells of the i-th row and j-th column. Therefore, there are $r(B - C_{ij}, k - 1)$ arrangements of k non-attacking rooks such that one rook is in c_{ij}. The number of arrangements of k rooks such that no rook is in c_{ij} is simply $r(B - c_{ij}, k)$. Thus we deduce the equality

$$r(B, k) = r(B - c_{ij}, k) + r(B - C_{ij}, k - 1) \tag{5}$$

For example,





B B-c_{12} B-C_{12}

$r(B, 1) = 5$	$r(B - c_{12}, 1) = 4$	$r(B - C_{12}, 0) = 1$
$r(B, 2) = 6$	$r(B - c_{12}, 2) = 4$	$r(B - C_{12}, 1) = 2$
$r(B, 3) = 1$	$r(B - c_{12}, 3) = 1$	$r(B - C_{12}, 2) = 0$

When (5) is substituted back into (2) we get a recursion relation

$$R(B) = R(B - c_{ij}) + x R(B - C_{ij}) \tag{6}$$

The following theorem, which is our main result, connects the numbers $r(B, k)$ with $p(G, k)$.

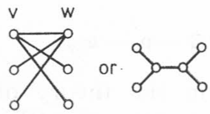
Theorem. There is a one-to-one correspondence between labelled bipartite graphs $G = G(B)$ with $a + b$ vertices and boards $B = B(G)$ with a rows and b columns, such that $p(G, k) = r(B, k)$ for all k.

Proof. Let us construct a labelled graph $G = G(B)$ with $a + b$ vertices v_1, $v_2, \ldots, v_a, w_1, w_2, \ldots, w_b$ by connecting the vertex v_i to w_j by an edge e_{ij} if and only if there is a cell c_{ij} in the board B. This graph is obviously bipartite since the vertices v_i (and also w_i) are not mutually connected.

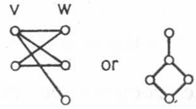
Now, according to the construction, two edges e_{ij} and e_{pq} are independent if and only if the cells c_{ij} and c_{pq} belong to different rows and different columns ($i \neq p$, $j \neq q$). Therefore the number of selections of k independent edges in G (i. e. $p(G, k)$) is equal to $r(B, k)$.

Corollary. $\varrho(B(G)) = \alpha(G(B))$.

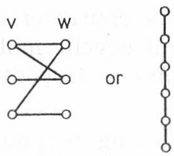
The graphs corresponding to the boards B_1, B_2, B_3 and B_4 are G_1, G_2, G_3 and G_4, respectively.



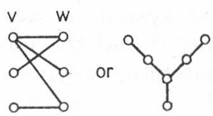
G1



G2



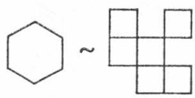
G3



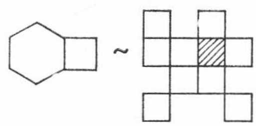
G4

The ϱ-polynomials of B_i are in the same time the matching polynomials of G_i, $i = 1, \ldots, 4$.

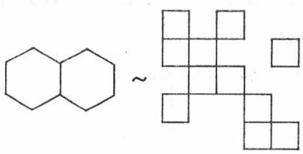
Because of the Theorem, the molecular graph of every alternant conjugated system can be presented in the form of a board. For instance, the molecular boards of benzene, benzcyclobutadiene and naphthalene are B_5, B_6 and B_7.



B5



B6



B7

It is clear that the board representation of alternant conjugated molecules is rather unusual from a chemists' point of view. Nevertheless, we think that the above given Theorem will be of some help even in theoretical chemistry because

(a) it connects two such diverse fields of science as the theory of aromaticity and rook theory and

(b) it enables the application of the numerous known results and proof techniques of rook theory.

In fact, it becomes clear that a great part of the results which were obtained for $\alpha(G)$ were previously known in rook theory. For example, when eqs. (5) and (6) are »translated« by means of our Theorem, one gets

$$p(G, k) = p(G - e_{ij}, k) + p(G - v_i - w_j, k - 1)$$

and

$$\alpha(G) = \alpha(G - e_{ij}) - \alpha(G - v_i - w_j)$$

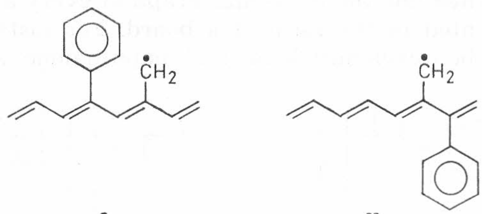
which are the basic recurrence relations in the theory of matching polynomials[5-10]. The proof[19] of the reality of the zeros of $\varrho(B)$ was just a proof of the reality of the zeros of the matching polynomial of bipartite graphs.

ON A CONJECTURE ABOUT MATCHING POLYNOMIALS

If a conjugated system is acyclic, then its characteristic and matching polynomials coincide[8-10] and therefore isospectral acyclic molecules necessarily also have equal matching polynomials. Examples of isospectral acyclic molecular graphs can be found in[21,22].

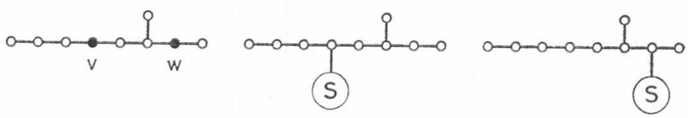
It was recently conjectured[3] that the matching polynomial can be used for discriminating between planar isospectral cyclic molecules. This conjecture is not true.

There exist pairs of cyclic conjugated systems with both characteristic and matching polynomials equal. *I* and *II* are examples of such molecules.



I II

Using an idea of Schwenk[23] it is not difficult to design as many such examples as desired. One of the possible construction procedures is the following.



G G′ G″

Notice that the vertices v and w in the graph G have the property $\alpha(G - v) = \alpha(G - w)$. Therefore, every pair of molecular graphs of the type G', G'' (where S stands for an arbitrary fragment) must have both characteristic and matching polynomials equal.

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SAŽETAK

Neke napomene o polinomu sparivanja i njegovim nulama

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Polinom sparivanja (koji se naziva još i aciklički i referentni polinom) otkrivan je u kemiji, fizici i matematici najmanje šest puta. Pokazano je da je polinom sparivanja svakog bikromatskog grafa identičan topovskom polinomu izvjesne ploče. Prikazane su osnove o teoriji topovskog polinoma[17]. Također je ukazano na činjenicu da se pomoću polinoma sparivanja ne mogu u općem slučaju razlikovati planarne izospektralne molekule.

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