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THE MATCHING POLYNOMIAL

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Abstract

The matching polynomial is a combinatorial mathematical structure which was recently discovered in theoretical chemistry within a novel approach to aromaticity. [5,6] The main, presently known properties of the matching polynomials are exposed.
The relation between the characteristic polynomial of a graph and matching polynomial is presented. Recurrence relations for matching polynomials are derived. All matching polynomials have real zeros. Identities are established between matching polynomials and certain special functions (Chebyshev, Hermité, Laguerre polynomials).

There are numerous graphic polynomials, i.e. polynomials which are associated with graphs. Such are, for example, the chromatic, the distance, the characteristic polynomial etc. Every graphic polynomial depends on particular properties of the graph and, thus, reflects the graph structure.

The graphic polynomials are useful in graph theory because they often enable the determination of properties of, and relations between graphs by means of algebraic methods.

The graphic polynomial which will be studied in the present paper and which is named "the matching polynomial" was introduced relatively recently. Hower, within a period of only few years it was independently discovered by a number of researchers.

In 1971 Hosoya [1] defined the "Z-counting polynomial" as

$$Q(G,\ X) = \sum_{k=0}^{m} p(G,\ k)\ X^{k} \qquad (1)$$

He used this polynomial for characterizing the topological nature of structural isomers of saturated hydrocarbons and their thermodynamic properties. [1,2] The meaning of the quantities p(G, k) will be explained later.

In 1972 Heilmann and Lieb [3] in apaper on the theory of monomer-dimer systems in statistical physics discussed the poperties of a polynomial, which was in fact identical with the later introduced mathing polynomial $\alpha(G,\ X)$. Heilmann and Lieb used no name for their polynomial.

It is an intriguing fact that this important work, although published in an easily available journal, seems to be not noticed by other researchers in the same field until fall 1978.

In 1975 the cocept of the "acyclic polynomial" was developed within a new theory of aromaticity. [4,5] This polynomial has been defined as

$$\alpha(G,\ X) = \sum_{k=0}^{m} (-1)^{k}\ p(G,\ k)\ X^{n-2k} \qquad (2)$$

The relation between the polynomials (1) and (2) is obvious: $X^n\, Q(G,\, -X^{-2}) = \alpha(G,\, X)$.

Few months later Aihara [6] independently discovered a similar approach to aromaticity. His "reference polynomial" turned out to be identical with the previously introduced acyclic polynomial. (The papers [4,5] were submitted for publication in November 1975 while the paper [6] was received in the journal in June 1976.)

In 1977 Farrell [7] defined and investigated the "matching polynomial" of a graph, which again coincides with $\alpha(G,\, X)$.

Throughout the present paper we shall accept this latter name for $\alpha(G,\, X)$. The reasons for this will become obvious during the following discussion.

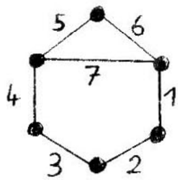
The fact that the matching polynomial is important in chemistry is nowadays well established and documented in a number of papers dealing with the theory of both saturated [1,2,8] and cojugated [4-6,9-19] hydrocarbons. Recently Aihara applied matching polynomials for describing the three dimensional aromaticity of boranes. [20] The fact that matching polynomials possess also a variety of properties of certain mathematical significance and intrinsic beauty is less familiar to the scientists being active in the field of mathematical chemistry. In the present paper we shall expose the most important known mathematical properties of matching polynomials, including a few new theorems and observation. Further results on this topic can be found elsewhere. [3,7,21-23]

Let G be a graph with n vertices and m edges. The vertices of G will be labeled by $v_1, v_2, \ldots, v_n$, while the edge connecting the vertices v_r and v_s is denoted by e_{rs}.

Definition 1. A subgraph of G possessing 2 k ($k \geq 1$) vertices v_{i_1} and v_{i_2} ($i=1,\ldots,k$) and k edges $e_{i_1 i_2}$ ($i=1,\ldots,k$) is called a k-matching in the graph G. The number of distinct k-matchings in G is denoted by p(G, k).

Of course, p(G, k) is equal to the number of selections of k independent edges in G. It is both convenient and consequent to define p(G, 0) = 1 for all graphs G.

We shallcall p(G, k) the k'th matching number of the graph G. Matching numbers play the central role in the whole theory of matching polynomials. Therefore we shall illustrate their calculation on the example of the graph G_a, possessing 6 vertices (n=6) and 7 edges (m=7). The edges of G_a are labeled by 1,2,...,7.



G_a

Case of k=1. One can select any edge, hence $p(G_a, 1) = 7$.

Case of k=2. Pairs of independent edges in G_a are: (1,3), (1,4),(1,5), (2,4), (2,5), (2,6), (2,7), (3,5), (3,6),(3,7), (4,6); hence $p(G_a, 2) = 11$.

Case of k=3. Triplets of independent edges which can be selected in G_a are: (1,3,5) and (2,4,6). Therefore $p(G_a, 3) = 2$.

Case of $k \geq 4$. It is not possible to select four or more independent edges in G_a. Thus, $p(G_a, 4) = p(G_a, 5) = \ldots = 0$.

The following properties of the matching numbers are immediate consequences of Definition 1.

1^o $p(G, 1) = m$

2^o $p(G, 2) = \frac{(m + 1)m}{2} - \frac{1}{2} (d_1^{\,2} + d_2^{\,2} + \ldots + d_n^{\,2})$

where d_i is the degree of the vertex v_i of G.

3^o If n is even, then $p(G, n/2)$ is equal to the number of one-factors of G.

4^o $p(G, k) = 0$ if $k > n/2$

5^o $p(G,k) = 0 \Rightarrow p(G, k+1) = 0$

6^o $p(G,k) = 1 \Rightarrow p(G, k+1) = 0$

Recently Schwenk proved [24] that for every graph G a number $K = K(G)$ can be determined, such that

$$p(G, 1) \leq p(G, 2) \leq \ldots \leq p(G, K) \geq p(G, K+1) \geq p(G, K+2) \geq \ldots$$

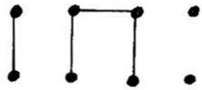
Definition 2. If G is a graph with n vertices and m edges, then its matching polynomial is denoted by $\alpha(G)$ or $\alpha(G, X)$ and is given by eq. (2).

For example, the matching polynomial of G_a reads $\alpha(G_a) = X^6 - 7X^4 + 11X^2 - 2$.

The characteristic polynomial $\phi(G,X)$ of a graph is the characteristic polynomial of its adjacency matrix. [25] The following important statement is an explanation why the name "acyclic" is sometimes attributed to the polynomial (G, X).

A graph is said to be acyclic if it contains no cycles. Hence, for example, G_b and G_c are acyclic graphs, but G_a is not.

G_b



G_c

Theorem 1 The matching polynomial of a graph G coincides with the characteristic polynomial of G,

$$\alpha(G, X) = \phi(G,X)$$

if, and only if G is an acyclic graph.

This result is a proper consequence of Definition 2 and the well known Sachs theorem. [25 - 27] In fact, Sachs proved [26] that

$$\phi(G, X) = \sum_{k=0}^{m} (-1)^k \, p(G, k) \, X^{n-2k}$$

if, and only if G is acyclic. The same result can be found also in a number of later publications.[28 - 30]

If G is composed of two disjoint components G_1 and G_2, then we shall write $G = G_1 \dot{+} G_2$

Theorem 2 $$\alpha(G_1 \dot{+} G_2) = \alpha(G_1)\, \alpha(G_2)$$

Proof

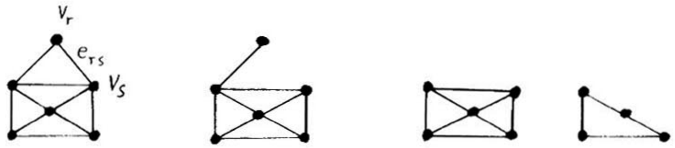
One can select a k-matching in G so that j of its edges belong to G_1 and k-j of its edges belong to G_2 (j=0,1,...,k). There are $p(G_1, j)\, p(G_2, k-j)$ such selections and, of course

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

Substitution of this relation back into eq. (2) yields Th.2.

<u>Corollary 2.1.</u> $\alpha(G_1 \dot{+} G_2 \dot{+} \ldots \dot{+} G_j) = \alpha(G_1)\,\alpha(G_2) \ldots . \alpha(G_j)$

Let e_{rs} be an arbitrary edge of G incident to the vertices v_r and v_s. We define now the subgraphs $G-e_{rs}$, $G-v_r$ and $G-v_r-v_s$. The subgraph $G - e_{rs}$ is obtained by deletion of the edge e_{rs} from G. The subgraph $G - v_r$ is obtained by deletion of the vertex v_r from G. Similarly, $G-v_r-v_s = (G-v_r)-v_s$.
For example,



G_d $\qquad$ G_d-e_{rs} $\qquad$ G_d-v_r $\qquad$ $G_d-v_r-v_s$

<u>Theorem 3.</u> Let e_{rs} be an arbitrary edge of G. Then the following recurrence relation holds.

$$\alpha(G) = \alpha(G-e_{rs}) - \alpha(G-v_r-v_s)$$

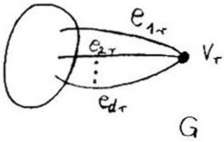
<u>Proof</u>
Among the selections of k-matchings in G there are $p(G-e_{rs}, k)$ selections which do not contain the edge e_{rs} and there are $p(G-v_r-v_s, k-1)$ selections which do contain e_{rs}.
Therefore,

$$p(G, k) = p(G-e_{rs}, k) + p(G-v_r-v_s, k-1)$$

which substituted back into eq. (2) yields Th.3.

Theorems 2 and 3 are rather important in practice, when the actual evaluation of the matching polynomials is required. [1,2, 4-6]

Let the edges e_{1r}, e_{2r}, ..., e_{dr} be incident to the vertex v_r.



Corollary 3.1.

$$\alpha(G) = X\,\alpha(G-v_r) - \sum_{j=1}^{d} \alpha(G-v_j-v_r) \tag{3}$$

Proof

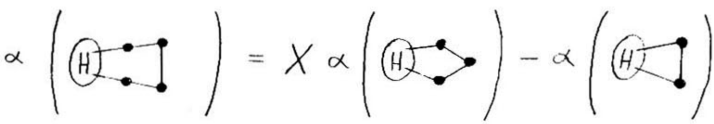
We apply Th.3 successively to the edges e_{1r}, e_{2r}, ..., e_{dr}

$$\begin{aligned}\alpha(G) &= \alpha(G-e_{1r}) - \alpha(G-v_1-v_r)\\ &= \alpha(G-e_{1r}-e_{2r}) - \alpha(G-v_1-v_r) - \alpha(G-v_2-v_r) = \ldots\\ \ldots &= \alpha(G-e_{1r}-e_{2r}-\ldots-e_{dr}) - \sum_{j=1}^{d} \alpha(G-v_j-v_r)\end{aligned}$$

From Th.2 we have $\alpha(G-e_{1r}-e_{2r}-\ldots-e_{dr}) = X\,\alpha(G-v_r)$ since the matching polynomial of an isolated vertex is simply X.

In the case of d= 0, i.e. when v_r is an isolated vertex in G, Cor. 3.1 reads simply $\alpha(G) = X\,\alpha(G-v_r)$.
If v_r is a vertex of degree one, we set d=1 in Cor. 3.1 and obtain the following result.

Corollary 3.2. [22] For H being an arbitrary subgraph,



Let us partition the edges e_{jr} (which are incident to the vertex v_r) into two groups: $\left\{e_{1r},\ldots,e_{tr}\right\}$ and $\left\{e_{t+1,r},\ldots e_{dr}\right\}$.
An analogous reasoning which led to Cor.3.1 gives

$$\alpha(G) = \alpha(G-e_{1r}-\ldots-e_{tr}) - \sum_{j=1}^{t} \alpha(G-v_j-v_r) \tag{4}$$

$$\alpha(G) = \alpha(G-e_{t+1,r}-\ldots-e_{dr}) - \sum_{j=t+1}^{d} \alpha(G-v_j-v_r) \tag{5}$$

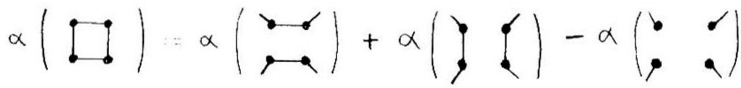
Combining eqs. (3)-(5) we deduce

<u>Corollary 3.4.</u> [22]

$$\alpha(G) = \alpha(G-e_{1r}-\ldots-e_{tr}) + \alpha(G-e_{t+1,r}-\ldots-e_{dr}) - \alpha(G-e_{1r}-\ldots-e_{dr})$$

A specialization of this result is the following

<u>Corollary 3.5.</u> [22]



A spanning subgraph of a graph G is a subgraph possessing all the vertices of G.
Note that the subgraphs $G-e_{1r}-\ldots-e_{tr}$, $G-e_{t+1,r}-\ldots-e_{dr}$ and $G-e_{1r}-\ldots-e_{dr}$ are obtained by deletion of some ed ges from G, but possess the same vertices as G; hence they are spanning subgraphs of G.

Now, according to Cor. 3.4 we can express the matching polynomial of G in terms of matching polynomials of its certain spanning subgraphs. If the application of Cor. 3.4

is repeated a sufficient number of times, one can express the matching polynomial of a graph G as a linear combination of matching polynomials of its acyclic spanning subgraphs F_j.

$$\alpha(G) = \sum_j a_j \alpha(F_j)$$

where a_j are non-negative integers. Since the spanning subgraphs F_j are acyclic, we can apply Th.1. This results in

Theorem 4.

$$\alpha(G) = \sum_j a_j \phi(F_j)$$

In graph spectral theory [25] the following identity is known for the first derivative of the characteristic polynomial of a graph.

$$\frac{d}{dX} \phi(G, X) = \sum_{r=1}^{n} \phi(G-v_r, X) \qquad (6)$$

We show now that an analogous result holds also for matching polynomials.

Corollary 4.1.

$$\frac{d}{dX} \alpha(G, X) = \sum_{r=1}^{n} \alpha(G-v_r, X)$$

Proof From Th. 3 we have

$$\alpha(G-v_r) = \sum_j a_j \phi(F_j-v_r)$$

Since the right side of this equation depends solely on characteristic polynomials, we can apply eq. (6). Thus

$$\sum_{r=1}^{n} \alpha\,(G-v_r) = \sum_{j} a_j \sum_{r=1}^{n} \phi\,(F_j-v_r) =$$

$$\sum_{j} a_j \frac{d}{dX} \phi\,(F_j) = \frac{d}{dX} \sum_{j} a_j\, \phi(F_j) = \frac{d}{dX}\alpha(G)$$

The zeros of $\alpha(G, X)$ are of certain importance in chemistry. [4-6, 9-20] They have been calculated (using computer routines) for a large number of graphs. The following important result was proved by Heilmann and Lieb [3], but was long time not recognized by chemists.

Theorem 5. All the zeros of matching polynomials of all graphs are real.

The same authors proved two additional properties of the zeros of the matching polynomials.

Theorem 6. [3] Let $X_1(G) \geq X_2(G) \geq \ldots \geq X_n(G)$ be the zeros of $\alpha(G)$ and $X_1(G-v) \geq X_2(G-v) \geq \ldots \geq X_{n-1}(G-v)$ the zeros of $\alpha(G-v)$, where v is an arbitrary vertex of G. Then the zeros of $\alpha(G-v)$ interlace the zeros of $\alpha(G)$, viz.

$$X_1(G) \geq X_1(G-v) \geq X_2(G) \geq X_2(G-v) \geq \ldots \geq X_{n-1}(G-v) \geq X_n(G); \quad (7)$$

Theorem 7. [3] If the graph G possesses a Hamiltonian path which starts at the vertex v, then the inequalities (7) are strict, i.e.

$$X_1(G) > X_1(G-v) > X_2(G) > X_2(G-v) > \ldots > X_{n-1}(G-v) > X_n(G)$$

Corollary 7.1. If the graph G possesses a Hamiltonian path (or, of course, a Hamiltonian cycle), then all the zeros of $\alpha(G)$ are mutually distinct.

Theorems 5 and 6 were recently proved independently by Godsil and Gutman.[31,32] One should note that the both available proofs of the reality of the zeros of the matching polynomials [3,31,32] are based on mathematical induction. Therefore, freely spoken, we know that Theorem 5 is true, but not "why" it holds and which are the graph theoretical "reasons" for its validity. From a combinatorial point of view, the matching polynomial is only one among many other possible polynomials of analogous structure. Bur only $\alpha(G)$ possesses the distinguished property that all its zeros are real.

Further investigations are, therefore, necessary in order to elucidate the relations between the combinatorial (i.e. graph theoretical) nature of $\alpha(G)$ and its algebraic properties. Some preliminary results along these lines are recently obtained by Schaad et al. [33]

We demonstrate now the properties of the matching polynomials of some special graphs. In particular, we show how these polynomials are related to certain special functions of mathemathical physics.[34]

Let P_n, C_n and K_n be the path, the cycle and the complete graph with n vertices. Let $K_{a,b}$ be the bicomplete graph with a+b vertices ($a \geqslant b$).

Theorem 8. Let T_n and U_n be the Chebyshev functions of the first and second kind; let He_n and H_n be the two standard forms of the Hermité polynomials; let L_n and L_n^k be the Laguerre and the generalized Laguerre polynomials, respectively. [34] Then the following identities hold.

$$\alpha(C_n, 2X) = 2\, T_n(X) \tag{8}$$

$$\sqrt{1 - X^2}\, \alpha(P_n, 2X) = U_{n+1}(X) \tag{9}$$

$$\alpha(K_n, X) = He_n(X) \tag{10}$$

$$2^{n/2} \alpha(K_n, 2X^2) = H_n(X) \tag{11}$$

$$\alpha(K_{aa}, X) = (-1)^a\, L_a(X^2) \tag{12}$$

$$\alpha(K_{a,b}, X) = (-1)^b\, X^{a-b}\, L_b^{a-b}\, (X^2) \tag{13}$$

Proof From Cor. 3.2 it follows that

$$\alpha(P_n) = X\, \alpha(P_{n-1}) - \alpha(P_{n-2})$$

while from Cor. 3.3 we gain an analogous relation

$$\alpha(C_n) = X\, \alpha(C_{n-1}) - \alpha(C_{n-2})$$

These recursion relations are closely similar to those valid for Chebyshev functions. [34] After making this observation it is not difficult to establish eqs. (8) and (9).

Since $K_n - v_r = K_{n-1}$ and $K_n - v_r - v_s = K_{n-2}$ for an arbitrary vertex v_r and an arbitrary edge e_{rs} of K_n, we deduce from Cor. 3.1,

$$\alpha(K_n) = X\, \alpha(K_{n-1}) - (n-1)\, \alpha(K_{n-2})$$

which is just the recursion relation for Hermité polynomials $He_n(X)$. [34] It is then easy to verify eqs. (10) and (11).

Eqs. (12) and (13) are obtained in an analogous manner.

Th. 8 confirms once again that the acyclic polynomial is a reasonably chosen mathematical structure. It also indicates a new and remarkable connection between graph theory and theory of special functions.

The above presented relations can be utilized in two different ways. First, eqs. (8-13) enable a new combinatorial interpretation of various special functions. Second, one can apply graph theoretical arguments and proof techniques in order to make the mathematical manipulations with special functions less complicated.

We shall illustrate this latter possibility by the following two examples. For an arbitrary vertex v, $C_n - v = P_{n-1}$. Form Cor. 4.1 we deduce then

$$\frac{d}{dX} \alpha(C_n, X) = n\,\alpha(P_{n-1}, X),$$

which combined with the identities (8) and (9) results in

$$U_n(X) = \frac{\sqrt{1 - X^2}}{n} \frac{d}{dX} T_n(X)$$

The bicomplete graph $K_{a,a}$ has the properties $K_{a,a} - v_r = K_{a,a-1}$ and $K_{a,a} - v_r - v_s = K_{a-1,a-1}$ for arbitrary adjacent vertices v_r and v_s. Then application of Cor.3.1 gives

$$\alpha(K_{a,a}) = X\,\alpha(K_{a,a-1}) - a\,\alpha(K_{a-1,a-1}) \qquad (14)$$

which is equivalent to the relation (15) between Laguerre polynomials.

$$L_a = a\,L_{a-1} - X\,L^{1}_{a-1} \qquad (15)$$

From eq. (14) one gains

$$\alpha(K_{a+1,\,a+1}) = X\,\alpha(K_{a+1,\,a}) - (a+1)\,\alpha(k_{a,a}) =$$

$$= X\,\left[X\,\alpha(K_{a,a}) - a\,\alpha(K_{a,a-1})\right] - (a+1)\alpha(K_{a,a})$$

and therefrom

$$\alpha(K_{a+1,\ a+1}) = (X^2 - 2a - 1)\ \alpha(K_{a,a}) - a^2\ \alpha(K_{a-1,\ a-1})$$

which immmediately results in a recurrence relation (16).

$$L_{a+1} = (2a + 1 - X)\ L_a - a^2\ L_{a-1} \tag{16}$$

It seems to be not simple to deduce eqs (15) and (16) using standard methods of mathematical analysis.

- X - X - X -

The author hopes that the results exposed in the present paper justified his belief that the matching polynomial is a quantity not only important in th eoretical chemistry, but also relevant from the point of view of pure mathematics. It is to be expected that further interesting results in this field will be obtained in the future.

After this paper has been presented on the Bremen Conference in summer 1978, a number of additional properties of the matching polynomial were discovered and/or came to the author's attention. Also a large number of new papers on the chemical application of $\alpha(G)$ were published in the meantime. Therefore the present paper was completely rewritten in March 1979.

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