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A NOVEL APPROACH TO GRAPH POLYNOMIALS

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A number of graph polynomials (matching, characteristic, permanental, μ-polynomial) and their generalizations can be expressed by means of a differential operator, associated with the graph.

Graph polynomials play an autstanding role in mathematical chemistry and, in particular, in chemical graph theory [1-3]. In the last few years the research in this field was so vigorous that only in the period 1980-1985 about 600 chemical papers were published on graph polynomials and closely related issues [4]. Bearing this in mind it is somewhat surprising that there still are some quite general mathematical properties of (chemically interesting) graph polynomials which have so far escaped the attention of both mathematicians and mathematical chemists. In the present paper we point out a few such properties and, in particular, demonstrate a new way in which a variety of graph polynomials can be expressed in a remarkably uniform way. Furthermore, the present paper is (to the authors' knowledge) the first time that a differential operator is employed as a mathematical tool in dealing with graph polynomials. Our results thus reveal certain hitherto unnoticed analytical properties of these polynomials.

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Let G be a graph and let its vertices be labeled by $1,2,\ldots,n$. A graph is completely determined by the specification of the connectedness of its vertices. This information is often presented in the form of the adjacency matrix $\underline{\underline{A}}$, whose (r,s)-entry is equal to unity if the vertices r and s are adjacent, and is equal to zero otherwise. Another, less common way to determine the graph G is to introduce n variables $x_1,x_2,\ldots,x_n$ and to construct a differential operator $\mathcal{D}$

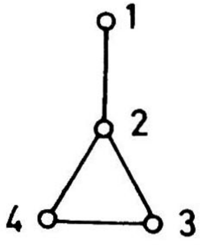
$$\mathcal{D} = \sum_{\substack{r \text{ adj } s \\ r < s}} \frac{\partial^2}{\partial x_r \, \partial x_s} \quad .$$

Throughout this paper we shall frequently refer to the product of the variables $x_1,x_2,\ldots,x_n$ and denote this product by X :

$$X = \prod_{i=1}^{n} x_i \quad .$$

Then it is clear that also $\mathcal{D}X$ characterizes the graph G up to isomorphism.

Consider as an example the graph G_1



G_1

$$X = x_1 \cdot x_2 \cdot x_3 \cdot x_4$$

Then

$$\mathcal{D} = \frac{\partial^2}{\partial x_1 \, \partial x_2} + \frac{\partial^2}{\partial x_2 \, \partial x_3} + \frac{\partial^2}{\partial x_2 \, \partial x_4} + \frac{\partial^2}{\partial x_3 \, \partial x_4}$$

and consequently,

$$\mathcal{D}X = x_3 \cdot x_4 + x_1 \cdot x_4 + x_1 \cdot x_3 + x_1 \cdot x_2 \quad .$$

Examine now the expression on the right-hand side of the latter equation. It contains four summands, which means that G_1 has four edges. The first summand is the product $x_3 \cdot x_4$ and since the variables x_1 and x_2 are missing from it, we can conclude that the vertices 1 and 2 are adjacent. The second, third and fourth product terms contain the information that also the vertex pairs (2,3), (2,4) and (3,4), respectively, are adjacent. This completely determines G_1.

In the present paper we shall be concerned with certain graph polynomials [4].

The matching polynomial [5,6] is defined as

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

where m(G,k) is the number of k-matchings of G, that is the number of ways in which k mutually non-incident edges can be chosen in G. We further introduce a closely related polynomial

$$\alpha^+(G,x) = \sum_k m(G,k)\, x^{n-2k} \quad .$$

The characteristic polynomial [2,5] of a graph G is just the characteristic polynomial of its adjacency matrix:

$$\phi^-(G,x) = \det(x\,\underline{I} - \underline{A}) \quad .$$

Here $\underline{I}$ is the unit matrix of order n.

The permanental polynomial [5,7] is

$$\phi^+(G,x) = \mathrm{per}(x\,\underline{I} + \underline{A})$$

where per stands for the permanent.

We define the generalized characteristic and permanental polynomials in the following manner. Let $\underline{X}$ be a diagonal matrix of order n, whose diagonal entires are the variables $x_1, x_2, \ldots, x_n$. Then

$$\phi^-(G,x_1,x_2,\ldots,x_n) = \det(\underline{X} - \underline{A})$$

$$\phi^+(G,x_1,x_2,\ldots,x_n) = \mathrm{per}(\underline{X} + \underline{A}) \quad .$$

Evidently, the above generalized quantities are linear functions of each x_i, i=1,2,...,n. By choosing $x_1 = x_2 = \cdots = x_n = x$ they reduce to $\phi^-(G,x)$ and $\phi^+(G,x)$, respectively. It is not difficult to see that $\phi^-(G,x_1,x_2,\ldots,x_n)$ and $\phi^+(G,x_1,x_2,\ldots,x_n)$ determine the graph G up to isomorphism.

DIFFERENTIAL OPERATOR REPRESENTATION OF THE MATCHING POLYNOMIAL

We first prove a relation for the matching numbers m(G,k), which is the basis for all results given in the present paper.

Theorem 1. If $x_1 = x_2 = \cdots = x_n = 1$, then

$$m(G,k) = (1/k!)\, \mathcal{D}^k X \quad .$$

Proof. One should observe that $\frac{\partial^{2k} X}{\partial x_{i_1} \partial x_{i_2} \cdots \partial x_{i_{2k}}}$ is equal to zero whenever not all indices $i_1, i_2, \ldots, i_{2k}$ are mutually distinct. Bearing in mind the definition of the operator $\mathcal{D}$, this means that $i_1, i_2, \ldots, i_{2k}$ must be the end-vertices of k mutually non-incident edges of G. Whence $\mathcal{D}^k X$ consists of a sum of terms, each corresponding to a selection of k non-incident edges of G. By setting $x_1 = x_2 = \cdots = x_n = 1$, each summand will be equal to unity.

There exist k! different ways to generate a summand corresponding to a given choice of k non-incident edges. Therefore by setting $x_1 = x_2 = \cdots = x_n = 1$ into $\mathcal{D}^k X$ we obtain a quantity which is k! times the number of distinct selections of k non-incident edges in G, i.e. m(G,k). □

Theorem 1 has a few interesting consequences. They are obtained by taking into account that

$$\sum_k (1/k!)\, \mathcal{D}^k = \exp(\mathcal{D})$$

and

$$\sum_k (-1)^k (1/k!)\, \mathcal{D}^k = \exp(-\mathcal{D}) \quad .$$

The Hosoya index [2,8] of a hydrocarbon is equal to the sum of all the matching numbers of the corresponding molecular graph.

Corolarry 1.1. If Z is the Hosoya index of a molecular graph G, then for $x_1 = x_2 = \cdots = x_n = 1$,

$$Z = \exp(\mathcal{D})\, X \quad .$$

Corollary 1.2. For $x_1 = x_2 = \cdots = x_n = x$,

$$\alpha^{\pm}(G,x) = \exp(\pm\mathcal{D})\ X \quad .$$

The above result motivates us to define the generalized matching polynomials $\alpha^{+}(G,x_1,x_2,\ldots,x_n)$ and $\alpha^{-}(G,x_1,x_2,\ldots,x_n)$ as

$$\alpha^{+}(G,x_1,x_2,\ldots,x_n) = \exp(\mathcal{D})\ X$$

$$\alpha^{-}(G,x_1,x_2,\ldots,x_n) = \exp(-\mathcal{D})\ X \quad .$$

That this is a reasonable choice is seen from the fact that $\alpha^{\pm}(G,x_1,x_2,\ldots,x_n)$ and $\phi^{\pm}(G,x_1,x_2,\ldots,x_n)$ coincide if and only if G is an acyclic graph. Thus the well-known [5,6] relation between the matching and the characteristic/permanental polynomial is valid also for their generalized versions.

We now point at three further properties of the generalized matching polynomial.

Theorem 2. Let q be a non-zero constant and $x_i/q = y_i$, i=1,2, ...,n. Then

$$\exp(\pm q^2\ \mathcal{D})\ X = q^n\ \alpha^{\pm}(G,y_1,y_2,\ldots,y_n) \quad .$$

Proof. Theorem 2 follows immediately from the definition of the operator $\mathcal{D}$. □

Corollary 2.1. If $x_1 = x_2 = \cdots = x_n = qx$, then

$$\exp(\pm q^2\ \mathcal{D})\ X = q^n\ \alpha^{\pm}(G,x) \quad .$$

Corollary 2.2. If $x_1 = x_2 = \cdots = x_n = q$, then

$$\exp(q^2\ \mathcal{D})\ X = q^n\ Z \quad .$$

Theorem 3.

$$\alpha^{\pm}(G,x_1,x_2,\ldots,x_n) = \prod_{\substack{r\ \mathrm{adj}\ s \\ r < s}} \left(1 \pm \frac{\partial^2}{\partial x_r\ \partial x_s}\right) X \quad .$$

Proof. In order to prove Theorem 3 recall that double differentiation of X with respect to any x_i , i=1,2,...,n, yields zero. Therefore,

$$\exp(\pm\mathcal{D})\ X = \prod_{\substack{r \text{ adj } s \\ r < s}} \exp\left(\pm\frac{\partial^2}{\partial x_r\ \partial x_s}\right) X =$$

$$= \prod_{\substack{r \text{ adj } s \\ r < s}} \left(1 \pm \frac{\partial^2}{\partial x_r\ \partial x_s} + \frac{1}{2}\ \frac{\partial^4}{\partial^2 x_r\ \partial^2 x_s} \pm \cdots\right) X =$$

$$= \prod_{\substack{r \text{ adj } s \\ r < s}} \left(1 \pm \frac{\partial^2}{\partial x_r\ \partial x_s}\right) X \quad .$$

Theorem 3 follows now from the definition of the generalized matching polynomials. □

Theorem 4.

$$\exp(\mp\mathcal{D})\ \alpha^{\pm}(G,x_1,x_2,\ldots,x_n) = X \quad .$$

Proof. We arrive at the above identity by recalling that the ring of all differential operators (in many variables) is associative. Therefore $\exp(\mathcal{D})\ \exp(-\mathcal{D}) = \exp(-\mathcal{D})\ \exp(\mathcal{D}) \equiv 1$. □

DIFFERENTIAL OPERATOR REPRESENTATION OF THE CHARACTERISTIC AND PERMANENTAL POLYNOMIAL

Consider a graph G which possesses cycles. Let Z_a be a cycle of G and let $i_1,i_2,\ldots,i_z$ be the vertices of G, belonging to Z_a. Hence the size of Z_a is z.

Define the operator $\mathcal{Z}_a$ as

$$\mathcal{Z}_a = \frac{\partial^z}{\partial x_{i_1}\ \partial x_{i_2}\ \ldots\ \partial x_{i_z}}$$

and another operator

$$\mathcal{C} = 2 \sum_a \mathcal{Z}_a$$

where the summation embraces all the cycles of the graph G. If G is acyclic, then $\mathcal{C} \equiv 0$.

We note in passing that

$$\exp(\pm\mathcal{C})\ X = \prod_a (1 \pm 2\ \mathcal{Z}_a)\ X$$

which can be deduced in an analogous manner as Theorem 3.

Theorem 5. Let $H = C + \mathcal{D}$. Then

$$\exp(\pm H)\ X = \phi^{\pm}(G,x_1,x_2,\ldots,x_n) \quad .$$

Proof. Theorem 5 is deduced by a similar reasoning as Theorem 1, taking into account the Sachs formula [2]. □

Corollary 5.1.

$$\exp(\pm C)\ \alpha^{\pm}(G,x_1,x_2,\ldots,x_n) = \phi^{\pm}(G,x_1,x_2,\ldots,x_n)$$

$$\exp(\mp C)\ \phi^{\pm}(G,x_1,x_2,\ldots,x_n) = \alpha^{\pm}(G,x_1,x_2,\ldots,x_n) \quad .$$

Corollary 5.2.

$$\exp(\mp H)\ \phi^{\pm}(G,x_1,x_2,\ldots,x_n) = X \quad .$$

DIFFERENTIAL OPERATOR REPRESENTATION OF THE μ-POLYNOMIAL

The μ-polynomial has been introduced [9] as a means by which the theory of the characteristic and the matching polynomial can be unified. Its definition can be found elsewhere [2,9,10].

The μ-polynomial depends on a vector $\underline{t} = (t_1,t_2,\ldots,t_r)$, where the parameter t_a is associated with the cycle Z_a of the graph G. The choice $t_a = 0$ for all a (i.e. $\underline{t} = \underline{0}$) reduces the μ-polynomial to $\alpha^-(G,x)$.

Instead of the operator C we now have to consider its generalization $C(\underline{t}) = 2 \sum_a t_a Z_a$. Then the following result can be shown to hold.

Theorem 6. Let $H(\underline{t}) = C(\underline{t}) + \mathcal{D}$. Then for $x_1 = x_2 = \cdots = x_n = x$,

$$\mu(G,\underline{t},x) = \exp[-H(\underline{t})]\ X \quad .$$

Corollary 6.1. For $x_1 = x_2 = \cdots = x_n = x$,

$$\mu(G,\underline{t},x) = \exp[-C(\underline{t})]\alpha^-(G,x_1,x_2,\ldots,x_n) \quad .$$

Corollary 6.2. For $x_1 = x_2 = \cdots = x_n = x$,

$$\mu(G,\underline{t},x) = \exp[C(\underline{1}-\underline{t})]\phi^-(G,x_1,x_2,\ldots,x_n) \quad .$$

Proof. Recall that $C = C(\underline{t}) + C(\underline{1}-\underline{t})$ and apply Corollary 5.1. □

From the above results is fairly evident that, in full analogy with $\alpha^{\pm}(G,x_1,x_2,\ldots,x_n)$ and $\phi^{\pm}(G,x_1,x_2,\ldots,x_n)$, one can introduce the two generalized forms of the μ-polynomial:

$$\mu^{+}(G,\underline{t},x_1,x_2,\ldots,x_n) = \exp[H(\underline{t})]\ X$$

$$\mu^{-}(G,\underline{t},x_1,x_2,\ldots,x_n) = \exp[-H(\underline{t})]\ X \quad .$$

The following properties of the generalized μ-polynomial are direct consequences of its definition:

$$\mu^{\pm}(G,\underline{0},x_1,x_2,\ldots,x_n) = \alpha^{\pm}(G,x_1,x_2,\ldots,x_n)$$

$$\mu^{\pm}(G,\underline{1},x_1,x_2,\ldots,x_n) = \phi^{\pm}(G,x_1,x_2,\ldots,x_n) \quad .$$

Whether the generalized μ-polynomial possesses other, non-trivial, mathematical properties and whether it can be applied in chemical (or other) investigations, remains to be established in the future.

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