Electronic Journal of Graph Theory and Applications **7** (1) (2019), 189–205

Electronic Journal of
Graph Theory and Applications

The cycle (circuit) polynomial of a graph with double and triple weights of edges and cycles

Vladimir R. Rosenfeld

Mathematical Chemistry Group, Department of Marine Sciences
Texas A&M University at Galveston, Galveston 77553–1675, USA; and
Department of Computer Science and Mathematics
Ariel University, Ariel 4070000, Israel

vladimir_rosenfeld@yahoo.com

Abstract

Farrell introduced the general class of graph polynomials which he called the *family* polynomials, or F-polynomials, of graphs. One of these is the *cycle*, or *circuit*, polynomial. This polynomial is in turn a common generalization of the characteristic, permanental, and matching polynomials of a graph, as well as a wide variety of statistical-mechanical partition functions, such as were earlier known.

Herein, we specially derive weighted generalizations of the characteristic and permanental polynomials requiring for calculation thereof to assign double (res. triple) weights to all Sachs subgraphs of a graph. To elaborate an analytical method of calculation, we extend our earlier differential-operator approach which is now employing operator matrices derived from the adjacency matrix. Some theorematic results are obtained.

Keywords: cycle (circuit) polynomial, Sachs graph method, weighted edges and cycles
Mathematics Subject Classification: C05C31, 32W99, 92E10, 94C15
DOI: 10.5614/ejgta.2019.7.1.15

Received: 14 January 2017, Revised: 6 February 2019, Accepted: 1 March 2019.

1. Introduction

Farrell [1] introduced the general class of graph polynomials which he called the *family* polynomials, or F-polynomials, of graphs. One of these is the *cycle*, or *circuit*, polynomial which is in turn a common generalization of the characteristic, permanental, and matching polynomials of a graph, as well as a wide variety of statistical-mechanical partition functions, such as were earlier known.

Owing to numerous applications in Hückel's simple method of linear combination of atomic orbitals (LCAO), the characteristic polynomial (of the adjacency matrix) of a molecular graph has appeared in chemistry. This polynomial can also be computed using the Sachs graph method, dealing with all vertex-disjoint covers of a graph with isolated vertices, lone edges, or simple cycles. Accordingly, all unoriented edges and unoriented proper cycles of a graph are used with the weights (-1) and (-2), respectively. If one instead uses the weights (+1) and (+2) for these subgraphs, one comes to the usual (but much less often applied) permanental polynomial of a graph. However, in the Pauling-Wheland resonance theory for a bipartite graph (or molecule), there arose also the need for a procedure to compute a generalized characteristic polynomial, associated with double weights (-2) and (-4) for edges and cycles, correspondingly, and, similarly, the generalized permanental polynomial, associated with double positive weights (+2) and (+4) for the same types of subgraphs, respectively. Here, we consider this subject on a slightly extended scale, since the Pauling-Wheland theory, as such, is chiefly a consumer of a selected group of 'intermediate-case' polynomials which are determined due to reweighting a certain number of cycles in covers, whereas the remaining cycles keep the usual weights. All this gives impetus to our present work which regards the subject in a larger context of instances of the cycle polynomial and the weights of edges and cycles.

For performing our analytical tasks, in the main part, we continue to elaborate our previous approach using the differential operators which represent Sachs subgraphs of a graph. But by now, such operators are used just implicitly, because we employ special operator matrices derived from the adjacency matrix. In the next parts, we consider these matters in a constant interaction with the general theory of F-polynomials.

2. Preliminaries

We start with giving some notions from the theory of graph polynomials.

2.1. The F- and B-polynomials of a graph

The graphs considered here are finite, may be directed, weighted; and may contain loops, *i. e.*, finite directed or undirected weighted pseudographs. A general class of graph polynomials was defined by Farrell [1]. These are called F-polynomials and are defined as follows. Let G be a graph and F a family of nonisomorphic connected subgraphs. An F-*cover* of G is a spanning subgraph of G, in which every component is a member of F. One also might define $F(G)$ as the family of subgraphs of G each of which is isomorphic to a member of F, and take an F-cover to be a set of subgraphs with every component in $F(G)$. Let us associate with each member α of F

an indeterminate or weight w_α. The weight of a cover C denoted by $w(C)$, is the product of the weights of its components. Then, the F-*polynomial* is

$$F(G; \mathbf{w}) = \sum w(C)\,, \tag{1}$$

where the summation is taken over all the F-covers of G, and where $\mathbf{w}$ is a vector of the indeterminates w_α.

Throughout this paper, we denote the vertex (or node) set of G by $V(G)$ and assume that $|V(G)| = p$, unless otherwise specified. Also, if G is labeled, we associate with the i-th vertex of G the special weight x_i $(i \in \{1, 2, \ldots, p\})$, where x_i is an indeterminate in addition to any weights for loops at i; this results in an extended recorded version $F(G; \mathbf{x}, \mathbf{w})$ of the F polynomial. We use the notation $F(G; \mathbf{x})$, for $F(G; \mathbf{x}, \mathbf{w})$, when all the variables, except the x_i's, are replaced by 1's. If we replace all x_i's, in $F(G; \mathbf{x})$, with the single variable x, then the resulting polynomial in x is denoted by $F(G; x)$, and called the *simple* F-*polynomial* of G.

If every nonnode member of F consists of exactly one block, then we call the corresponding class of F-polynomials, *block polynomials*, or B-*polynomials* [2–4], for short. We also write $B(G; \mathbf{w})$ for $F(G; \mathbf{w})$, in order to indicate this property of the members of F [2–4]. Notice that if we take F to be a family of cycles, then every nonnode member of F is a block. This is also true when F is the family of cliques. Thus, both the circuit (or cycle) polynomial and clique polynomial (see [2]) are examples of block polynomials. We therefore classify all the special circuit polynomials, for example the matching, characteristic, and permanental polynomials, as B-polynomials.

It should be noticed that often the families which give rise to B-polynomials consist of graphs which are characterized by the number of vertices, and that specific weights w_j are associated simply to the number of vertices. And in this circumstance, w_j $(j \in \{1, 2, \ldots, p\})$ is not associated to an isolated vertex j but rather the weight of a j-cycle. The resulting B-polynomial then contains monomials which totally describe the covers. In this general F-polynomial, the vector of weights is $\mathbf{w} = (w_1, w_2, \ldots)$. Observe that if F is the family of stars or paths, then every member of F is characterized by the number of nodes. However, stars and paths are not blocks and so do not give rise to B-polynomials.

The stimulus to investigate the B-polynomials stems from the fact that they are often encountered in many problems in (pure)mathematics, as well as in various applications. It is interesting to know about mutual and hereditary relations among different graph polynomials. For instance, the matching polynomial is a generalization of the so-called acyclic polynomial, which was defined independently (see [2]). The same matching polynomial yields, under certain substitutions, the chromatic polynomial for certain classes of graphs, and also a whole group of its relatives (see [2]), as well. The classical rook polynomial (see [2]) is yet another relative of the matching polynomial.

Notice that the most general F-polynomial is the subgraph polynomial (see [2]), since it enables us to derive, in principle, any other F-polynomial. However, the subgraph polynomial is not a B-polynomial. So, there exist other classes of F-polynomials; *e. g.*, see [2], wherein the so-called *articulation node polynomials* (or A-*polynomials*, for short) are introduced.

Now we shall specially consider some instances of the circuit polynomial.

2.2. The circuit (cycle) polynomial of a graph

The circuit (cycle) polynomial $C(U;\mathbf{w})$ of an undirected graph U was introduced by Farrell [5] (see [6, 7]). The notion of this polynomial was generalized in [2–4] for an arbitrary graph G. Herein, we give the third definition of it [4], which is, nevertheless, tantamount to that of [2, 3], where the circuit polynomial was regarded in quite a different way, as a specific case of the F-polynomial. In order to indicate the distinction between Farrell's original polynomial $C(U;\mathbf{w})$ and the one that is used in the present paper, we denote the latter by $P(U;\mathbf{x};\mathbf{w})$, where $\mathbf{x} = (x_1, x_2, \ldots, x_p)$ is, by analogy with $\mathbf{w}$, the vector of indeterminates (see [3, 4]).

Many properties of the polynomial in question can be considered from a matrix-theoretic standpoint. Let $A = [a_{ij}]_{i,j=1}^{p}$ be the adjacency matrix of a graph G. Let further $A^* = [a^*_{ij}]_{i,j=1}^{p} = (A + w_1 X)$ be an auxiliary matrix, where X is a diagonal matrix, whose on-diagonal entries are indeterminates $x_1, x_2, \ldots, x_p$, consecutively. One can define the *circuit* (*cycle*) *polynomial* $P(G;\mathrm{x};\mathrm{w})$ *of a graph* G as follows [6]:

$$P(G;\mathbf{x};\mathbf{w}) := \sum_{\sigma\in S_p}\left(\prod_{i=1}^{p} a^*_{i\sigma i}\prod_{j=2}^{p} w_j^{\omega_j(\sigma)}\right) = \sum_{\sigma\in S_p}\prod_{\substack{i=1\\ j=2}}^{p} a^*_{i\sigma i} w_j^{\omega_j(\sigma)}, \tag{2}$$

where $a^*_{i\sigma i}$ is the respective entry of A^*; $\omega_j(\sigma)$ is the number of cycles of length j in a permutation σ; and the sum ranges over all the $p!$ permutations σ of a symmetric group S_p. (Recall that σi is the image of an index $i \in I = \{1, 2, \ldots, p\}$, obtained under the action of a permutation σ on I).

The polynomial $C(U;\mathbf{w})$ of an undirected graph U, introduced by Farrell (see [5, 6]), is a specific case of $P(U;\mathbf{x};\mathbf{w})$, *viz.*:

$$C(U;\mathbf{w}) = P(U;\mathbf{x};\mathbf{w})\Big|_{x_i=1;\, w_j\to\frac{w_j}{2}\quad (i\in\{1,2,\ldots,p\};j\in\{3,4,\ldots,p\})}, \tag{3}$$

where $w_j \to \frac{w_j}{2}$ denotes the substitution of $\frac{w_j}{2}$ for w_j.

We mention in passing one relation for $P(U;\mathbf{w})$, connected to the enumerative theory of Pólya (see [4, 8, 9]). Let K_p be a complete (di)graph with p vertices. Then,

$$P(K_p;\mathbf{w}) = p!Z(S_p;V;w_1,w_2,\ldots,w_p), \tag{4}$$

where $Z(S_p;V;\mathbf{w})$ is the cycle index of the symmetric group S_p faithfully acting on a vertex set $V = V(K_p)$ ($|V| = p$) of K_p (see [8, 9]).

The circuit polynomial $P(G;\mathbf{x};\mathbf{w})$ has, as its specific cases, the *generalized permanental polynomial* $\phi^+(G;\mathbf{x})$, *generalized characteristic polynomial* $\phi^-(G;\mathbf{x})$, and two *generalized matching polynomials* $\alpha^+(G;\mathbf{x})$ and $\alpha^-(G;\mathbf{x})$ [4, 10, 11]; *viz.*:

$$\phi^+(G;\mathbf{x}) = \mathrm{per}(X+A) = P(G;\mathbf{x};\mathbf{w})\Big|_{w_i=1\quad (i\in\{1,2,\ldots,p\})}, \tag{5}$$

$$\phi^-(G;\mathbf{x}) = \det(X-A) = P(G;\mathbf{x};\mathbf{w})\Big|_{w_1=1;\, w_i=-1\quad (i\in\{2,3,\ldots,p\})}, \tag{6}$$

$$\alpha^+(G;\mathbf{x}) = P(G;\mathbf{x};\mathbf{w})\Big|_{w_1=w_2=1;\, w_i=0\quad (i\in\{3,4,\ldots,p\})}, \tag{7}$$

$$\alpha^-(G;\mathbf{x}) = P(G;\mathbf{x};\mathbf{w})\Big|_{w_1=1;\, w_2=-1;\, w_i=0\quad (i\in\{3,4,\ldots,p\})}. \tag{8}$$

It is worth noting that the weight (see [2–4]) of a loop at a vertex i of G entails an entry a_{ii} of A. Also, one could give the edges $\{i, j\}$ weights x_{ij}, as in Klein [12]. And also, a numerous statistical-mechanical partition functions are realized as special cases (including several of the cases already mentioned).

Since there are more possibilities to devise other such polynomials with the adjective "generalized", we here confine ourselves to only the above instances, to avoid any confusion. Recall the *simple circuit polynomial* $P(G; x)$ is a one-variable case of it, with an italicized x in lieu of **x**, *viz.*:

$$P(G; x) = P(G; \mathbf{x})\,\big|_{x_i = x \quad (i\in\{1,2,\ldots,p\})}\ , \tag{9}$$

while the variables $w_1, w_2, \ldots, w_p$ may or may not be reduced (it depends on the context).

The notation $P(G; \mathbf{x}; \mathbf{w})$ or any of its reduced-variable forms hereafter stand for every possible instance of it at once; the reader can reinterpret any of general solutions for any specific circuit polynomial that needed in – the permanental, characteristic, matching cases. (Moreover, some other B-polynomials can have the same properties, *e. g.*, the clique polynomial; see [2].) Here, we recall that a widely studied and widely used instance of the circuit polynomial is the *simple characteristic polynomial* $\phi^-(G; x)$; see [13–15] (for mathematicians) and [16–19] (for chemists) for monographs concerning it.

We want also to note that the existence of formulae (5) through (8) allows us not to employ herein the Sachs graph method (see [13]) mentioned in the Abstract, as such. For this, there are at least three reasons. First, this method easily follows from (2), if one adapts it for an undirected graph U, where there are always allowed two oppositely directed cycles passing through the same sets of vertices and edges. Just for this reason, the weights of proper cycles (of lengths ≥ 3) are taken in his approach to be 2 for deriving the permanental polynomial $\phi^+(U; x)$ of an undirected graph U and -2 for its characteristic polynomial $\phi^-(U; x)$, rather than 1 and -1, respectively, as in (5) and (6) for a directed graph G. Secondly, (5) and (6) utilize directly the adjacency matrix A of G and are thereby universally true for both undirected and directed graphs; thus, there is no need in confining our reasoning by dealing only with undirected graphs, as the classical form of the Sachs method does. Third, we are not planning to confine ourselves by considering only the (usual) permanental and characteristic polynomials, but want to study, in perspective, a wide set of cycle polynomials associated with cycles having arbitrary integral weights – above all, double and triple ones, with respect to those which are used in the Sachs method.

Thus, in addition to the usual polynomials $\phi^+ = \phi_1^+$ and $\phi^- = \phi_1^-$ above, we study special normalized polynomials ϕ_m^+ and ϕ_m^- $(m \geq 2)$ associated with m-fold weights mw_j $(j \geq 2)$ of edges and cycles, substituted for respective weights w_j in (5) and (6). In other words, these are

$$\phi_m^+(G; \mathbf{x}) := \sum_{\sigma\in S_p} \prod_{\substack{i=1\\ j=2}}^{p} a_{i\sigma i}^{*} m^{\omega_j(\sigma)} = P(G; \mathbf{x}; \mathbf{w})\,\big|_{w_1=1;\, w_j=m \ (j\in\{2,3,\ldots,p\})}\ , \tag{10}$$

$$\phi_m^-(G; \mathbf{x}) := \sum_{\sigma\in S_p} \prod_{\substack{i=1\\ j=2}}^{p} a_{i\sigma i}^{*} (-m)^{\omega_j(\sigma)} = P(G; \mathbf{x}; \mathbf{w})\,\big|_{w_1=1;\, w_j=-m \ (j\in\{2,3,\ldots,p\})}\ , \tag{11}$$

with corresponding simple forms $\phi_m^+(G; x)$ and $\phi_m^-(G; x)$; *cf.* (2).

In order to borrow our previous results from [10, 11], we have to consider some actions of differential operators associated with c-cycles $(c \geq 1)$ of a (di)graph G. For this purpose, we turn to the next subsection.

2.3. Using differential operators for calculating polynomials ϕ^+ and ϕ^-

Here, we need to expound the differential-operator approach earlier applied by us [10, 11] to calculation of polynomials $\phi^+(G;\mathbf{x})$, $\phi^-(G;\mathbf{x})$, $\alpha^+(G;\mathbf{x})$, and $\alpha^-(G;\mathbf{x})$. It may also be applied to calculation of any F-polynomial of G.

Let F be the family of all c-cycles $(c \geq 1)$ of a digraph G, where cases of $c = 1$ and $c = 2$ correspond to loops and edges, respectively, $c = 3$ to triangles, *et seq.*. Consider an arbitrary c-cycle $\alpha \in F$ with vertex set $V(\alpha) = \{j_1, j_2, \ldots, j_c\}$, where vertices are identified with indices that number them, for short. Associate to α the following differential operator:

$$D(\alpha) := w_c \frac{\partial^c}{\partial x_{j_1} \partial x_{j_2} \cdots \partial x_{j_c}} \quad (c \geq 1). \tag{12}$$

Recall that the product $D_1 \cdot D_2$ of two differential operators in p variables is defined as follows:

$$D_1 \cdot D_2 = \frac{\partial^{\beta_1+\beta_2+\cdots+\beta_p}}{\partial x_1^{\beta_1} \partial x_2^{\beta_2} \cdots \partial x_p^{\beta_p}} \cdot \frac{\partial^{\gamma_1+\gamma_2+\cdots+\gamma_p}}{\partial x_1^{\gamma_1} \partial x_2^{\gamma_2} \cdots \partial x_p^{\gamma_p}} = \frac{\partial^{\beta_1+\beta_2+\cdots+\beta_p+\gamma_1+\gamma_2+\cdots+\gamma_p}}{\partial x_1^{\beta_1+\gamma_1} \partial x_2^{\beta_2+\gamma_2} \cdots \partial x_p^{\beta_p+\gamma_p}}, \tag{13}$$

where superscripts β_i and γ_i $(i \in \{1, 2, \ldots, p\})$ are arbitrary nonnegative integers (see also below). The set of all bare (unweighted) differential operators comprises a commutative, associative differential ring D, with a zero $\hat{0}$ and unit $\hat{1}$, which is extended to form an algebra WD over the field W of weights:
(i) $(w_1 D_1 + w_2 D_2) \in \mathsf{WD}$;
(ii) $(w_1 D_1 \cdot w_2 D_2) = w_1 w_2 (D_1 \cdot D_2) \in \mathsf{D}$ for all $D_1, D_2 \in \mathsf{WD}$;
(iii) $(w_1 + w_2)D = w_1 D + w_2 D$ for all $w_1, w_2 \in \mathsf{W}$ and $D \in \mathsf{WD}$;
(iv) $1D = D$ for all $D \in \mathsf{WD}$ along with $w\hat{0} = \hat{0}$ and $\hat{0}w = 0$ for all $w \in \mathsf{W}$.
Note that $w\hat{1}$ can be identified as $w = \hat{1}w$ $(w \in w \in \mathsf{W})$ and, in essence, $\hat{1}$ is nothing else than the 0-th derivative $\frac{\partial^0}{\partial \xi^0}$ with respect to an arbitrary (dummy) variable ξ or simply 0-th differential ∂^0 with no variable at all (see also another trick later).

But some additional special characteristics arise in that the algebra acts as operators on the space of polynomials in $x_1, x_2, \ldots, x_n$. Then, $D \in \mathsf{WD}$ can act on $0 \in \mathsf{W}$, which can often replace $\hat{0}$ – but not always; $\hat{1} \in \mathsf{W}$ <u>cannot</u> generally be replaced with 1, except for $\hat{1}$ standing to the left of D, because for any differential operator $D \in \mathsf{D}$ we have $1D = D$, whereas $D1 = 0$ (since the differentiation of a constant always gives 0). Just this fact was not properly mentioned by us earlier in [10, 11], where correct final results were in some places accompanied with an incorrect notation 1 instead of the needed $\hat{1}$. We use below just $\hat{1}$ and, wherever possible, only legitimate manipulations that allow to replace it.

Now, we turn to the next section, where we derive new rigorous statements from known ones [10, 11].

3. The main part

The *multilinearity* (or *multiaffinity*) of F-polynomials $F(G;\mathbf{x},\mathbf{w})$, *i. e.*, linearity for each variable x_i ($i \in \{1,2,\ldots,p\}$) separately, plays a crucial role in our differential-operator method (see [10, 11]) to analytically generate these polynomials. Here, the following technical lemma, based on the very fundamentals of differential calculus, is crucial:

Lemma 1. *For all integers $s \geq 2$ and every variable $x_i \in \{x_1, x_2, \ldots, x_n\}$,*

$$\frac{\partial^s}{\partial x_i^s} x_i \equiv \hat{0} x_i = 0 \quad (s \geq 2). \tag{14}$$

Proof. It is self-evident. □

Employing the Lemma 1, Rosenfeld and Gutman [10, 11] obtained the following result (initially formulated for the characteristic, permanental, and matching polynomials but holding true for all F-polynomials). *Viz.*:

Lemma 2. *Let F be the family of all c-cycles ($c \in \{1,2,\ldots,p\}$) α of a digraph G, with weights w_c ($c = |V(\alpha)|$) and associated differential operators $D(\alpha)$, defined in (12). Then,*

$$P(G;\mathbf{x};\mathbf{w}) = \left[\prod_{\alpha\in F(G)} \left(\hat{1} + D(\alpha)\right)\right] \prod_{i=1}^{p} x_i, \tag{15}$$

where the first product embraces all c-cycles $\alpha \in F$ and the second does all vertex variables x_i ($i \in \{1,2,\ldots,p\}$); while weight-indeterminates w_c are all implicitly included in operators D.

Proof. Apparently, to each 'correct' F-cover in (15), which consists of disjoint components α, these corresponds a product of differential operators that contains just the first derivative with respect to each variable used in the cover and, thus, contributes to the L. H. S. of (15). On the contrary, on the R. H. S., each 'incorrect' F-cover must contain overlapping components α and is necessarily associated with differential operators containing derivatives of higher-than-first order. By virtue of the Lemma 1, the latter F-covers do not contribute to the L. H. S. of (15), which immediately affords the proof. □

We state here our first planned result, which is a generalizing corollary of the Lemma 2 for the case of the *normalized cycle polynomial* $P_m(G;\mathbf{x};\mathbf{w}) := P(G;\mathbf{x}; w_1, mw_2, \ldots, mw_p)$ ($m \geq 1$) with m-fold weights of all edges and all proper cycles (but not loops). *Viz.*:

Theorem 3. *Let F be a family of all c-cycles ($c \in \{1,2,\ldots,p\}$) α of a digraph G, with weights w_c ($c = |V(\alpha)|$) and associated differential operators $D(\alpha)$, defined in (12). Let also $P_m(G;\mathbf{x},\mathbf{w})$ be the normalized cycle polynomial of G, as above. Then,*

$$\begin{aligned} P_m(G;\mathbf{x};\mathbf{w}) &= \left[\prod_{\alpha^*\in F}\prod_{\alpha\in F} \left(\hat{1} + D(\alpha^*)\right)\left(\hat{1} + mD(\alpha)\right)\right] \prod_{i=1}^{p} x_i = \\ &\quad \left[\prod_{\alpha^*\in F}\prod_{\alpha\in F} \left(\hat{1} + D(\alpha^*)\right)\left(\hat{1} + D(\alpha)\right)^m\right] \prod_{i=1}^{p} x_i \quad (m \geq 1), \end{aligned} \tag{16}$$

where the first product in square brackets embraces all loops $\alpha^* \in F$, if any, and the second product embraces all other c-cycles $(c \in \{2, 3, \ldots, p\})$ $\alpha \in F$; the external product includes all variables x_i $(i \in \{1, 2, \ldots, p\})$, while weight-indeterminates w_c are all implicitly included in operators $D(\alpha)$.

Proof. With use of the Lemma 2, the first equality in (16) follows from definitions of $D(\alpha)$ (see (12)) and $P_m(G; \mathbf{x}, \mathbf{w})$, while the second equality holds by virtue of the Lemma 1, whence the overall proof is immediate. □

Earlier, we promised to tell of one "trick" that allows to substitute something for $\hat{1}$. Now, we can do this. To this end, we state here a modified version of Theorem 3, *viz.*:

Theorem 4. *Let F be a family of all c-cycles $(c \in \{1, 2, \ldots, p\})$ α of a digraph G, with weights w_c $(c = |V(\alpha)|)$ and associated differential operators $D(\alpha)$, defined in (12). Besides, let $P_m(G; \mathbf{x}, \mathbf{w})$ be the normalized cycle polynomial of G and ξ be a variable independent of x_i $(i \in \{1, 2, \ldots, p\})$. Then,*

$$\begin{aligned} P_m(G; \mathbf{x}; \mathbf{w}) \quad &= \quad \left\{ \left[\prod_{\alpha^* \in F} \prod_{\alpha \in F} \left(\frac{\partial}{\partial \xi} + D(\alpha^*) \right) \left(\frac{\partial}{\partial \xi} + mD(\alpha) \right) \right] \exp(\xi) \prod_{i=1}^{p} x_i \right\} \exp(-\xi) = \\ (m \geq 1) \quad & \quad \left. \left\{ \left[\prod_{\alpha^* \in F} \prod_{\alpha \in F} \left(\frac{\partial}{\partial \xi} + D(\alpha^*) \right) \left(\frac{\partial}{\partial \xi} + D(\alpha) \right)^m \right] \exp(\xi) \prod_{i=1}^{p} x_i \right\} \right|_{\xi = 0}, \end{aligned} \tag{17}$$

where the products are as in Theorem 3.

Proof. It is based on Theorem 3. Evidently, for all nonnegative integers s, $\frac{\partial^s}{\partial \xi^s} \exp(\xi) = \exp(\xi)$, which proves the first equality. The second follows from the fact that $\exp(\xi)|_{\xi=0} = \exp(0) = 1$. This gives the overall proof. □

Theorem 4 does not involve $\hat{1}$, as such, and employs different methods of representing the same operations. Note that such operations can directly be programmed for symbolic computations. But from the analytical point of view, the most elegant way to calculate the cycle polynomials using differential operators is embodied in the following lemma (see [10, 11]):

Lemma 5. *Let F be a family of all c-cycles $(c \in \{1, 2, \ldots, p\})$ of a graph G, with weights w_c $(c = |V(\alpha)|)$ and associated differential operators $D(\alpha)$, defined in (12). Then,*

$$P(G; \mathbf{x}; \mathbf{w}) = \left[\exp \left(\sum_{\alpha \in F} D(\alpha) \right) \right] \prod_{i=1}^{p} x_i, \tag{18}$$

where the summation ranges over all c-cycles $\alpha \in F$ and the weight-indeterminates w_c are all included in operators $D(\alpha)$.

Proof. Since $\exp(x) = 1+x+x^2/2+\cdots$, by virtue of Lemma 1, we have $[\exp(D(\alpha))]\prod_{i=1}^{p} x_i = \left[\hat{1} + D(\alpha)\right]\prod_{i=1}^{p} x_i$. Thus, the R. H. S. of (18) is equal to the R. H. S. of (15), which completes the proof. □

From Lemma 5, we may easily derive the following generalization:

Theorem 6. *Let F be a family of all c-cycles $(c \in \{1, 2, \ldots, p\})$ of a graph G, with weights w_c $(c = |V(\alpha)|)$ and associated differential operators $D(\alpha)$, defined in (12). Let also $P_m(G; \mathbf{x}, \mathbf{w})$ be the normalized cycle polynomial of G. Then,*

$$P_m(G; \mathbf{x}; \mathbf{w}) = \left\{\exp\left[\left(\sum_{\alpha^* \in F} D(\alpha^*)\right) + m\left(\sum_{\alpha \in F} D(\alpha)\right)\right]\right\}\prod_{i=1}^{p} x_i \quad (m \geq 1), \tag{19}$$

where the α^*, α summation ranges are as for the corresponding product ranges in Theorem 3, and the i product is as there also.

Proof. It follows from Lemma 5 and the definition of $P_m(G; \mathbf{x}; \mathbf{w})$. □

A practically important remark concerning all results above touches the 'norm' m which determines the generalized cycle polynomial $P_m(G; \mathbf{x}, \mathbf{w})$ with scaled weights. The very definition does not demand that m must necessarily be an integer or a number at all. But really, all formulae involving a fragment of type $(\hat{1} + D(\cdots))^m$ become impracticable under m which is not a (positive) integer, though remaining theoretically true. In particular, such are the last sides of (16) and (17). The formulae above that contain a fragment of type $mD(\cdots)$ can be used with an arbitrary m. This remark serves also as an introduction to the next part of the section where we have to consider different results involving special operator matrices, which encompass only two values $m = 2, 3$ and for which generalizations for subsequent values of m are (yet) unknown. A reason for discussing such narrow findings here is motivated by a hope to practically utilize them further using symbolic-calculation programming packages like MuPAD, Matlab, Mathematica, and Maple. An unarguable advantage of such a narrower matrix-operator approach is that it demands to know just the adjacency matrix A of G, rather than the family F of all c-cycles $(c \in \{1, 2, \ldots, p\})$, which is unavoidable if one uses any of results above for computing the polynomial $P_m(G; \mathbf{x}, \mathbf{w})$. Nevertheless, formulae (15) through (19) may be used in deriving relationships between different sorts of polynomials, say, between the characteristic and permanental polynomials [10, 11] as well as for deriving general working algorithms using the recursion of polynomials (and graphs).

Let $\hat{I}$ be a diagonal matrix (of consistent size) whose on-diagonal entries are all $\hat{1}$'s and let $\hat{B} = [\hat{b}_{ij}]_{i,j=1}^{p}$ be a matrix with an entry $\hat{b}_{ij} = a_{ij}\sqrt{\partial^2/\partial x_i \partial x_j}$ $(\hat{b}_{ii} = a_{ii}\partial/\partial x_i)$, where a_{ij} is an x-independent entry of the (weighted) adjacency matrix A; and $\sqrt{\partial^2/\partial x_i \partial x_j}$ is a fractional derivative. We do not need to worry about any detailed definition of fractional derivative, but only note that they all commute, and that $\sqrt{\partial/\partial x_i} \cdot \sqrt{\partial/\partial x_i} = \partial/\partial x_i$. Since all the $\hat{b}_{ij}$ commute, one may speak of ordinary determinants and permanents of $\hat{B}$, or of $\hat{I} \pm \hat{B}$, or other polynomials of $\hat{B}$. In all such instances, whenever a factor $\sqrt{\partial/\partial x_j}$ arises from one $\hat{b}_{ij}$ there is also another factor $\sqrt{\partial/\partial x_j}$ arising from some $\hat{b}_{jk}$, so that only integer powers of $\partial/\partial x_j$ arise; and our operations map from the ring D back into itself. Rosenfeld and Gutman [11] proved the following two results:

www.ejgta.org

Lemma 7. *Let $\phi^{-}(G;\mathbf{x})$ be the characteristic polynomial of a (weighted) (di)graph G and let $\hat{B}$ be the matrix operator defined above. Then,*

$$\phi^{-}(G;\mathbf{x}) = \left[\det\left(\hat{I}-\hat{B}\right)\right]\prod_{i=1}^{p} x_i. \tag{20}$$

Lemma 8. *Let $\phi^{+}(G;\mathbf{x})$ be the permanental polynomial of a (weighted) (di)graph G and let $\hat{B}$ be the matrix operator defined above. Then,*

$$\phi^{+}(G;\mathbf{x}) = \left[\operatorname{per}\left(\hat{I}+\hat{B}\right)\right]\prod_{i=1}^{p} x_i. \tag{21}$$

Taking into account the relationships between the characteristic polynomial $\phi^{-}(G;\mathbf{x})$ and the permanental polynomial $\phi^{+}(G;\mathbf{x})$ [10, 11], they derived also the following common corollary of Lemmas 7 and 8 (see Theorem 8 and Corollary 8.1 in [11]):

Corollary 8.1.

$$\phi^{+}(G;\mathbf{x}) = \left[\det\left(\hat{I}-\hat{B}\right)\right]^{-1}\prod_{i=1}^{p} x_i = \det\left(\hat{I}-\hat{B}\right)^{-1}\prod_{i=1}^{p} x_i = \left[\det\left(\hat{I}+\hat{B}+\hat{B}^2+\cdots+\hat{B}^s\right)\right]\prod_{i=1}^{p} x_i\,, \tag{22}$$

where $s \le p$ is the maximum number of components α in F-covers of G.

Since all results for the characteristic and permanental polynomials can be written down in very similar forms, we consider below just universal statements which can easily embrace both cases. As a 'trial instance', we first present a convolution of Lemmas 7 and 8 into one statement, taking into account also the Corollary 8.1. *Viz.*:

Lemma 9. *Let $\phi^{\mp}(G;\mathbf{x})$ be a common notation for the characteristic (–) and permanental (+) polynomials of a (weighted) (di)graph G and let $\hat{B}$ be the matrix operator defined above. Then,*

$$\phi^{\mp}(G;\mathbf{x}) = \left[\det\left(\hat{I}-\hat{B}\right)\right]^{\pm 1}\prod_{i=1}^{p} x_i, \tag{23}$$

where the upper and lower signs correspond to the characteristic and permanental polynomial, respectively.

Although a repetitive action of matrix operators on the R. H. S.'s of (20) and (21) is already a true theoretical way to calculate respective polynomials $\phi_m^{-}(G;\mathbf{x})$ and $\phi_m^{+}(G;\mathbf{x})$, we want to derive special matrix operators that perform the double and triple action of the mentioned operators just for one application. Let $\hat{C} = [\hat{c}_{ij}]_{i,j=1}^{p}$ be another matrix with an entry $\hat{c}_{ij} = a_{ij}\partial/\partial x_i$, where a_{ij} is an entry of the (weighted) adjacency matrix A. We state here a result which is much the same in appearance to that of Lemma 9, *viz.*:

Lemma 10. *Let $\phi^{\mp}(G;\mathbf{x})$ be a common notation for the characteristic (–) and permanental (+) polynomials of a (weighted) (di)graph G and let $\hat{C}$ be the matrix operator defined above. Then,*

$$\phi^{\mp}(G;\mathbf{x}) = \left[\det\left(\hat{I} - \hat{C}\right)\right]^{\pm 1} \prod_{i=1}^{p} x_i, \tag{24}$$

where the upper and lower signs correspond to the characteristic and permanental polynomial, respectively.

Proof. It utilizes the same reasoning that was used in the case of Lemma 7 (see [11]). Let α be an arbitrary oriented h-cycle $(h \in \{1, 2, \ldots, p\})$ with circularly ordered vertices $j_1, j_2, \ldots, j_h$ or simply, without any loss of generality, vertices $1, 2, \ldots, h$. By definition of the matrix $\hat{C}$, the product $\hat{c}_{12}\hat{c}_{23}\cdots\hat{c}_{h1}$ is equal to $\partial^h/\partial x_1 \partial x_2 \cdots \partial x_h$, which is just $D(\alpha)$. Thus, indeed, the expansion of $\det(\hat{I} - \hat{C})$ results in an operator whose differential action on $\prod_{i=1}^{p} x_i$ is equivalent to a similar action of the operator $\left[\prod_{\alpha \in F}\left(\hat{1} + D(\alpha)\right)\right]$ on the R. H. S. of (15), provided that all weight-indeterminates w_h $(h \in \{1, 2, \ldots, p\})$ are determined consistently with a choice of either polynomial (ϕ^- or ϕ^+). Thus, we arrive at the proof. □

Let $\hat{X} = \operatorname{diag}\{a_{11}\frac{\partial}{\partial x_1}, a_{22}\frac{\partial}{\partial x_2}, \ldots, a_{pp}\frac{\partial}{\partial x_p}\}$ be a diagonal matrix. Adopting the fashion of Lemmas 9 and 10, we state here the first of results promised in the title of our paper, *viz.*:

Theorem 11. *Let $\phi_2^{\mp}(G;\mathbf{x})$ be a common notation for the normalized characteristic (–) and permanental (+) polynomials of a (weighted) (di)graph G and let $\hat{C}$ be the matrix operator defined above. Then,*

$$\phi_2^{\mp}(G;\mathbf{x}) = \left[\det\left(\hat{I} + \hat{X} - \hat{C} - \hat{C}^T\right)\right]^{\pm 1} \prod_{i=1}^{p} x_i, \tag{25}$$

where the upper and lower signs correspond to the normalized characteristic and permanental polynomial, respectively; the matrix $\hat{X}$ is introduced to avoid double weighting of loops; and $\hat{C}^T$ denotes the transpose of $\hat{C}$.

Proof. It utilizes the same reasoning that was used in Lemma 10 and Lemma 1. □

From a technical point of view, we need to derive here the following corollary which is very similar to the Corollary 8.1, *viz.*:

Corollary 11.1. *Let $\phi_2^{+}(G;\mathbf{x})$ be the generalized permanental polynomial, as above. Then,*

$$\phi_2^{+}(G;\mathbf{x}) = \left[\det\left(\hat{I} + \sum_{t=1}^{s}\left(\hat{C} + \hat{C}^T - \hat{X}\right)^t\right)\right] \prod_{i=1}^{p} x_i, \tag{26}$$

where $s \leq p$ is the maximum number of components α in F-covers of G, which can always be replaced by p (or any natural number $> s$), if s is undetermined.

We do not present herein all variations of results. Say, one may replace either $\hat{C}$ or $\hat{C}^T$ with $\hat{B}$ in (25) and (26), provided that the expansion of a thus obtained operator $[\cdots]$ neglects all members that contain fractional powers of any derivatives, *i. e.*, $\sqrt{\partial/\partial x_i}$. This circumstance helps us to state the second promised result, *viz.*:

Theorem 12. *Let $\phi_3^{\mp}(G;\mathbf{x})$ be a common notation for the normalized characteristic (–) and permanental (+) polynomials of a (weighted) (di)graph G and let $\hat{B}$ and $\hat{C}$ be the matrix operators defined above. Then,*

$$\phi_3^{\mp}(G;\mathbf{x}) = \left[\det\left(\hat{I} + 2\hat{X} - \hat{B} - \hat{C} - \hat{C}^T\right)\right]^{\pm 1} \prod_{i=1}^{p} x_i, \tag{27}$$

where the upper and lower signs correspond to the normalized characteristic and permanental polynomial, respectively; the matrix operator $2\hat{X}$ stands to avoid triple weighting of loops; and the condition is obeyed that the expansion of the operator $[\cdots]$ neglects all fractional differentials.

Proof. It uses the same reasoning that Lemma 10 and takes into account Lemma 1. □

The instances of Corollaries 8.1 and 11.1 would help the reader to introduce similarly the notation per instead of $\det^{-1}$ in (24)–(27).

Now, we perform one task simply to illustrate how our differential-operator approach may work. This also produces some rigorous statements but these are quite a facultative addition to the main results above which are *per se* selfcontained.

3.1. A case in point

To imitate practical tasks which may be performed in a similar way, introduce the following derivative polynomial:

$$Q(G;\mathbf{x};\mathbf{w}') := \sum_{\alpha\in F'} w'_\alpha P(G-\alpha;\mathbf{x};\mathbf{w}), \tag{28}$$

where $G-\alpha$ is the induced subgraph obtained by deleting the set $V(\alpha)$ of vertices, of a subgraph α, from G; the (two-fold) weight w'_α equals 2 for each edge and 4 for each undirected cycle (or 2 for each directed cycle, equivalently); and the sum ranges over the entire subfamily $F' \subseteq F$ of subgraphs, of F, which is F less all loops thereof, if any; $P(G;\mathbf{x};\mathbf{w}) \equiv \phi^+(G;\mathbf{x};\mathbf{w})$.

We need to recall the following known result of Farrell and Grell (due to Lemma 3 in [7]):

Lemma 13. *Let $C(G;\mathbf{w})$ be Farrell's cycle (circuit) polynomial (see [5; 6, 7] or above). Then,*

$$\frac{\partial C(G;\mathbf{w})}{\partial w_i} = \sum C(G-C_i;\mathbf{w}), \tag{29}$$

where the summation is taken over all the circuits C_i with a fixed number i ($i \in \{1,2,\ldots,p]$) of vertices.

To us, it is more convenient to utilize a more relevant form of their result, *viz.*:

Corollary 13.1. *Let $P(G;\mathbf{x};\mathbf{w})$ be the cycle (circuit) polynomial as above. Then,*

$$\frac{\partial P(G;\mathbf{x};\mathbf{w})}{\partial w_i} = \sum P(G - C_i;\mathbf{x};\mathbf{w}), \tag{30}$$

where the summation is taken over all the circuits C_i with a fixed number i ($i \in [1,p]$) of vertices.

Proof. Adding extra variables $x_1, x_2, \ldots, x_p$ to Farrell's set $w_1, w_2, \ldots, w_p$ in (29) does not infringe the trueness of the original statement. The passage from $C(G;\mathbf{x};\mathbf{w})$ to $P(G;\mathbf{x};\mathbf{w})$ is guaranteed by (3). Hence, the proof follows. □

The next technical corollaries are due to Corollary 13.1.

Corollary 13.2. *Let $P(G;\mathbf{x};\mathbf{w})$ be the cycle (circuit) polynomial as above. Then,*

$$w_i \frac{\partial P(G;\mathbf{x};\mathbf{w})}{\partial w_i} = \sum w_i P(G - C_i;\mathbf{x};\mathbf{w}), \tag{31}$$

where the summation is taken over all the circuits C_i with a fixed number i ($i \in \{1,2,\ldots,p\}$) of vertices.

Corollary 13.3. *Let $P(G;\mathbf{x};\mathbf{w})$ be the cycle (circuit) polynomial as above. Then,*

$$\sum_{\alpha \in F'} w_\alpha \frac{\partial P(G;\mathbf{x};\mathbf{w})}{\partial w_\alpha} = \sum_{\alpha \in F'} w_\alpha P(G - \alpha;\mathbf{x};\mathbf{w}), \tag{32}$$

where the summation is taken over all members (edges and cycles) of the subfamily $F' \subseteq F$.

This corollary derived for the polynomial $P(G;\mathbf{x};\mathbf{w}) = P_1(G;\mathbf{x};\mathbf{w})$ is generalized for the normalized polynomial $P_m(G;\mathbf{x};\mathbf{w}) = P(G;\mathbf{x};w_1, mw_2, \ldots, mw_p)$ as follows:

Corollary 13.4. *Let $P(G;\mathbf{x};\mathbf{w})$ be the cycle (circuit) polynomial as above. Then,*

$$\sum_{\alpha \in F'} w_\alpha \frac{\partial P_m(G;\mathbf{x};\mathbf{w})}{\partial w_\alpha} = \sum_{\alpha \in F'} m w_\alpha P_m(G - \alpha;\mathbf{x};\mathbf{w}), \tag{33}$$

where the summation is taken over all members (edges and cycles) of the subfamily $F' \subseteq F$.

Using an individual variable x_i ($i \in \{1,2,\ldots,p\}$) for each vertex of G (which is indicated by the vector $\mathbf{x} = (x_1, x_2, \ldots, x_p)$ above) allows us to utilize the form of differential operator $D(\alpha)$ (12) for alternatively determining $\rho_2^+(G;\mathbf{x};\mathbf{w})$ (*cf.* (28)). We state here the following:

Proposition 14. *Let $Q(G;\mathbf{x};\mathbf{w}')$ be the derivative polynomial as above. Then,*

$$Q(G;\mathbf{x};\mathbf{w}') = \sum_{j=2}^{p} w_j' \frac{\partial}{\partial w_j} P(G;\mathbf{x};\mathbf{w}) = 2\left[\sum_{\alpha \in F'} D(\alpha)\right] P(G;\mathbf{x};\mathbf{w}), \tag{34}$$

where the weights w_α are already implicitly included in operators $D(\alpha)$ (see (12)).

www.ejgta.org

Proof. The first equality follows from Corollary 13.4 (under $m = 2$). The second equality in (34) follows from that fact that $w'_j = 2w_j$ and $D(\alpha)\phi^+(G;\mathbf{x};\mathbf{w}) = \sum_{\alpha\in F'} w_\alpha \phi^+(G-\alpha;\mathbf{x};\mathbf{w})$. This gives the overall proof. □

We remind to the reader that, by definition, the weight-indeterminates w_j $(j \in \{2,3,\ldots,p\})$ in the notation of the polynomial $\phi^+(G;\mathbf{x};\mathbf{w}) = P(G;\mathbf{x};\mathbf{w})$ are all assigned to edges $(j = 2)$ and directed cycles $(j \geq 2)$ (*i. e.*, not undirected ones!). Bearing this in mind, introduce a derivative expression (to imitate a real physical task):

$$Q(G;\mathbf{w}') = \left[\frac{1}{P(G;\mathbf{w})}\left(\sum_{\alpha\in F'} w'_\alpha \frac{\partial}{\partial w_\alpha}\right) P(G;\mathbf{w})\right]_{\mathbf{w}=\mathbf{u}} = \left[\left(\sum_{\alpha\in F'} w'_\alpha \frac{\partial}{\partial w_\alpha}\right)\ln P(G;\mathbf{w})\right]_{\mathbf{w}=\mathbf{u}}, \tag{35}$$

where the vector $\mathbf{u}$ of weights depends (in an applied context) on the temperature of a physical system and obeys the condition $P(G;\mathbf{u}) = 1$; (35) turns out to be of a form appears in statistical mechanical and quantum mechanical cluster expansions (see [20]). Indeed, such a ratio for general weights is “additive” in the sense that $Q(G;\mathbf{w}') = Q(G_1;\mathbf{w}') + Q(G_2;\mathbf{w}')$ for a disjoint union $G = G_1 \oplus G_2$ of subgraphs G_1 and G_2 [20].

Apparently, when the graph G in (34) has no loops, the subfamily $F' = F$, and we can apply in (33) the summation over the entire family F. In order to determine $Q(G;\mathbf{w}')$ using operator matrices, we should first state the following lemma:

Lemma 15. *Let $\sum_{\alpha\in F} D(\alpha)$ be a weighted-operator sum as in (34). Then,*

$$2\sum_{\alpha\in F} D(\alpha) = \det\left(\sum_{t=1}^{s}\frac{1}{t}\left(\hat{C} + \hat{C}^T - \hat{X}\right)^t\right) \tag{36}$$

Proof. It follows from a simultaneous consideration of (18), (26), the fact that $\ln(1+x) = \sum_{t=1}^{\infty}\frac{1}{t}x^t$, and that only (the first) s terms in the sum on the R. H. S. of (36) give a nonzero contribution to the L. H. S. of it. □

Taking into account (26), (34), and (35), we state our final result:

Proposition 16. *Let $Q(G;\mathbf{w}')$ be the polynomial as above. Then,*

$$Q(G;\mathbf{w}') = \left.\frac{\left[\det\left(\sum_{t=1}^{s}\frac{1}{t}\left(\hat{C} + \hat{C}^T - \hat{X}\right)^t\right)\right]\left[\det\left(\hat{I} + \sum_{t=1}^{s}\hat{B}^t\right)\right]\prod_{i=1}^{p} x_i}{\left[\det\left(\hat{I} + \sum_{t=1}^{s}\hat{B}^t\right)\right]\prod_{i=1}^{p} x_i}\right|_{\mathbf{x}=\mathbf{u}}. \tag{37}$$

Notice also that our previous approach [10, 11] has already been implemented in symbolic computer codes and practically employed by Salvador *et al.* [21] and Cash [22] for computing the matching and permanental polynomials of molecular graphs.

4. Conclusions

As was already mentioned, an earlier instance of this differential-operator approach has been employed by other authors (as well as by ourselves) for calculating certain graph polynomials. One of the fields where this finds application is (mathematical) chemistry, wherein studying finite (molecular) graphs with a not too large number of vertices is constantly of use, and certain graph polynomials (may) play a very important role. In a broader crossdisciplinary context, a similar combined approach, involving also the Pólya cycle indicator as another sort of multivariate "graph" polynomials, is adapted for enumeration of substitutional isomers with restrictive mutual positions of ligands [23, 24].

By now, we can preliminarily state that a certain extension of the described differential operator method to integer values $m \geq 4$ is also possible. The generalized approach additionally involves an algorithm of finding all oriented simple paths of length m between every pair, j and k, of vertices in a (di)graph G. Such paths should also have differential-operator weights for each arc in them. Accordingly, an arc jk carries an operator weight $\partial/\partial x_j$ (alternatively, $\partial/\partial x_k$), while the weight $\hat{\zeta}_{jk}^{(m)}$ of an oriented path is the product of all arc weights therein (*i. e.*, a partial differential operator linear in each involved variable). The sum $\hat{\omega}_{jk}^{(m)} = \sum \hat{\zeta}_{jk}^{(m)}$ $(j, k \in \{1, 2, \ldots, p\})$ of the weights of all oriented simple paths, from a vertex j to a vertex k, determines an entry of an operator matrix $\hat{\Omega}^{(m)} = [\hat{\omega}_{jk}^{(m)}]_{j,k=1}^{p}$, which plays much the same role as the m-th power, $\hat{C}^m$, of the matrix $\hat{C}$ above. In particular, $\hat{\Omega}^{(m)} \prod_{j=1}^{p} x_j = \hat{C}^m \prod_{j=1}^{p} x_j$ (which is here just an illustration satisfying Lemma 1). A more detailed exposition will follow later.

Acknowledgments

We acknowledge the support of the Welch Foundation of Houston, Texas (through grant BD–0894) and the Ministry of Absorption of the State Israel (via fellowship "Shapiro").

[1] E.J. Farrell, On a general class of graph polynomials, *J. Comb. Theory B* **26** (1) (1979), 111–122.

[2] E.J. Farrell and V.R. Rosenfeld, Block and articulation node polynomials of the generalized rooted product of graphs, *J. Math. Sci. (Calcutta)* **11** (1) (2000), 35–47.

[3] V.R. Rosenfeld and M.V. Diudea, The block-polynomials and block-spectra of dendrimers, *Internet Electron. J. Mol. Des.* **1** (3) (2002), 142–156.

[4] V.R. Rosenfeld, The circuit polynomial of the restricted rooted product $G(\Gamma)$ of graphs with a bipartite core G, *Discrete Appl. Math.* **156** (2008), 500–510.

[5] E.J. Farrell, On a class of polynomials obtained from circuits in a graph and its application to characteristic polynomials of graphs, *Discrete Math.* **25** (1979), 121–133.

[6] E.J. Farrell and J.C. Grell, The circuit polynomial and its relation to other polynomials, *Carib. J. Math.* **2** (1/2) (1982), 15–24.

[7] E.J. Farrell and J.C. Grell, On reconstructing the circuit polynomial of a graph, *Caribb. J. Math.* **1** (3) (1983), 109–119.

[8] A. Kerber, *Algebraic Combinatorics via Finite Group Actions*, Wissenschaftsverlag, Manheim, Wein, Zürich, 1991.

[9] A. Kerber, *Applied Finite Group Actions*, Springer Verlag, Berlin, Heidelberg, New York, London, Raris, Tokyo, Hong Kong, Barcelona, Budapest, 1999.

[10] V.R. Rosenfeld and I. Gutman, A novel approach to graph polynomials, *Commun. Math. Comput. Chem (MATCH)* **24** (1989), 191–199.

[11] V.R. Rosenfeld and I. Gutman, On the graph polynomials of a weighted graph, *Coll. Sci. Papers. Fac. Kragujevac* **12** (1991), 49–57.

[12] D.J. Klein, Variation localized-site cluster expansions V. Valence-bond and Heisenberg models, *Mol. Phys.* **31** (3) (1976), 811–823.

[13] D.M. Cvetković, and H. Sachs, *Spectra of Graphs: Theory and Application*, Academic Press, Berlin (1980).

[14] D.M. Cvetković, M. Doob, I. Gutman, and A. Torgašev, *Recent Results in the theory of Graph Spectra*, North-Holland, Amsterdam (1988).

[15] D. M. Cvetković, P. Rowlinson, and S. Simić, *Eigenspaces of Graphs*. Series: Encyclopedia of Mathematics and Its Applications. Cambridge University Press, Cambridge (1997).

[16] A. Streitwieser, *Molecular Orbital Theory for Organic Chemists*, Wiley, New York (1961).

[17] E. Heilbronner, H. Bock, *Das HMO-Modell und seine Anwendungen*, Weinheim, Verlag Chemie (1968, 1970); English translation: E. Heilbronner, H. Bock, *The HMO Model and Its Application, Vols. 1–3*, Verlag Chemie, Weinheim (1970).

[18] A. Tang, Y. Kiang, G. Yan, S. Tai, *Graph Theoretical Molecular Orbitals*, Science Press, Beijing (1986).

[19] J.R. Dias, *Molecular Orbital Calculations Using Chemical Graph Theory*, Springer-Verlag, Berlin (1993).

[20] D.J. Klein and V.R. Rosenfeld, Forcing, freedom, and uniqueness in graph theory and chemistry, *Croat. Chem. Acta* **87** (1) (2014), 49–59.

[21] J.M. Salvador, K. Hernandez, A. Beltran, R. Duran, and A. Mactutis, Differential synthesis of the matching polynomial of C72-100, *J. Chem. Inf. Comput. Sci.* **38** (6) (1998), 1105–1110.

[22] G.G. Cash, A differential-operator approach to the permanental polynomial, *J. Chem. Inf. Comput. Sci.* **42** (5) (2002), 1132–1135.

[23] V.R. Rosenfeld and D.J. Klein, Enumeration of substitutional isomers with restrictive mutual positions of ligands. I. Overall counts, *J. Math. Chem.* **51** (1) (2013), 21–37.

[24] V.R. Rosenfeld and D.J. Klein, Enumeration of substitutional isomers with restrictive mutual positions of ligands. II. Counts with restrictions on (sub)symmetry, *J. Math. Chem.* **51** (1) (2013), 239–264.