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The circuit polynomial of the restricted rooted product $G(\Gamma)$ of graphs with a bipartite core G

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Abstract

As an instance of the B -polynomial, the circuit, or cycle, polynomial $P(G(\Gamma); \mathbf{w})$ of the generalized rooted product $G(\Gamma)$ of graphs was studied by Farrell and Rosenfeld [Block and articulation node polynomials of the generalized rooted product of graphs, *J. of Math. Sci. (India)* 11(1) (2000) 35–47] and Rosenfeld and Diudea [The block polynomials and block spectra of dendrimers, *Internet Electron. J. Mol. Design* 1(3) (2002) 142–156]. In both cases, the rooted product $G(\Gamma)$ was considered without any restrictions on graphs G and Γ . Herein, we present a new general result and its corollaries concerning the case when the core graph G is restricted to be bipartite.

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1. Introduction

As it was phrased in *Scientific American*, today is a nanotechnology gold rush. To the mathematical reader, it may be pleasant to recognize that mathematics (and, in particular, the theory of graph spectra) is also seeking to make its contribution to this interdisciplinary area [22,1–5,32,8–15,33,25,26,20,28]. The present paper continues the previous work [20,28] along these lines.

From the graph-theoretical point of view, there exists a number of molecular structures (or graphs) of high-tech interest that can be generated using the graphical construction called, in the mathematical literature, the generalized rooted product of graphs (see [20,28,6,21]). Here, first of all, of special practical significance are dendrimers [22,1–4,32,14,15], for which some authors also use other names (e.g., “bundled structures”, as in [5]).

As well as any other type of products relevant to chemical objects, the rooted product of molecular graphs contains combinatorial information that is useful for the (theoretical) chemist. Algebraically, this information can be represented in the form of respective graph polynomials of the molecular graph in question. One type of such polynomials (namely, the circuit polynomial) will be considered by us throughout this paper.

An algorithmic role of the results that will be discussed below can be clarified through recalling, as an example, the following situation. Creating complex dendritic molecules also foresees that the researcher would have suitable quantum-chemical (or any other) methods for estimating the energy levels of respective large molecules. A common tack is to utilize for this the simpler solutions that had been obtained for dendrimer’s core and monodendrons. Namely,

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this sort of calculation proposes mathematical results that follow below. However, we want to specially stress that that we shall, in fact, deal with the derivation of universal mathematical relationships for the circuit polynomial which are not based on any approximation that might follow from quantum-chemical or other calculational methods that can adapt them.

Now that we have briefly described the applied background of the paper, we need to focus upon a rigorous mathematical exposition of our specific task.

2. Preliminaries

We should 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 self-loops, i.e., finite directed or undirected weighted pseudographs. A general class of graph polynomials was introduced in Farrell [16]. These are called F -polynomials and are defined as follows. Let G be a graph and F a family of connected subgraphs of G . An F -cover of G is a spanning subgraph of G , in which every component is a member of F . Let us associate with each member α of F an intermediate 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

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

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 $x_i + b_i$ ($1 \leq i \leq p$), where x_i is an indeterminate and b_i is the sum of weights of all loops, if any, lying in a vertex i (see [29,30]). We use the notation $F(G; \mathbf{x})$, for $F(G; \mathbf{w})$, 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 will be denoted by $F(G; x)$, and called the *simple* 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* for short. We then write $B(G; \mathbf{w})$ for $F(G; \mathbf{w})$, in order to indicate this property of the members of F . 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. Therefore, both the circuit (or cycle) polynomial and clique polynomial (see [20]) are examples of block polynomials. We therefore classify all the special circuit polynomials, for example, the matching, characteristic, and permanent polynomials (see [33,6–13,25,26,19–21,28–30,16,17]), as B -polynomials.

It should be observed that the families which give rise to B -polynomials consist of graphs which are characterized by the number of vertices. Therefore, when general weights are to be assigned to the members of F , it is sufficient to associate with each member, of F , with n vertices the weight w_n . The resulting B -polynomial would therefore contain monomials which totally describe the covers. In this general F -polynomial, the vector of weights is $\mathbf{w} = (w_1, w_2, \dots, w_p)$. 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 mathematics, as well as in various applications outside of mathematics. 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 [20]). 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 [20]) as well. The classical rook polynomial (see [20]) is yet another relative of the matching polynomial.

Notice that the most general F -polynomial is the subgraph polynomial (see [20]), 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 [20], 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 [17] (see [19]). The notion of this polynomial was generalized in [20,28] for an arbitrary graph G . Herein, we shall give the third definition of it, which is, however, tantamount to that of [20,28], where the circuit polynomial was considered in quite a different way, as a specific case of the F -polynomial. In order to indicate the distinction between the original Farrell’s polynomial $C(U; \mathbf{w})$ and the one that will be used in the present paper, we shall denote the latter by $P(U; \mathbf{x}; \mathbf{w})$, where $\mathbf{x} = (x_1, x_2, \dots, x_p)$ is, by analogy with \mathbf{w} , the vector of indeterminates (see [28]).

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

$$P(G; \mathbf{x}; \mathbf{w}) := \sum_{\sigma \in S_p} \prod_{i=1}^p a_{i\sigma i}^* w_i^{\omega_i(\sigma)}, \tag{2}$$

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

The polynomial $C(U; \mathbf{w})$ of an undirected graph U , introduced by Farrell (see [17,19]), is a specific case of $P(U; \mathbf{x}; \mathbf{w})$, viz.:

$$C(U; \mathbf{w}) = P(U; \mathbf{x}; \mathbf{w})|_{x_i=1; b_i=0; w_j \rightarrow w_j/2} \quad (1 \leq i \leq p; 3 \leq j \leq p), \tag{3}$$

where $w_j \rightarrow w_j/2$ denotes the substitution of $w_j/2$ for w_j .

In general, if a graph G is directed (2) does not hold. We can mention in passing one ready result for $C(U; \mathbf{w})$, connected to the enumerative theory of Pólya (see [23,24]). Let K_p be a complete graph with p vertices. Then

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

where $Z(S_p; V; \mathbf{w})$ is the cycle indicator of a symmetric group S_p faithfully acting on a vertex set $V = V(K_p)$ ($|V|=p$) of K_p (see [23,24]).

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 $\alpha^-(G; \mathbf{x})$ [29,30], viz.:

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

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

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

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

It is worth noting that the weight b_i ($1 \leq i \leq p$) (see [20,28]) of a self-loop lying in a vertex i of G is thereby equal to an entry a_{ii} , of A , in case of $\phi^+(G; \mathbf{x})$ and $\alpha^+(G; \mathbf{x})$; however, b_i is equal to $-a_{ii}$ in case of $\phi^-(G; \mathbf{x})$ and $\alpha^-(G; \mathbf{x})$.

Apparently, there are more possibilities to devise other such polynomials with the adjective “generalized”; herein, we shall confine ourselves only to 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 a lieu of \mathbf{x} , viz.:

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

while the variables w_1, w_2, \dots, 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 form will hereafter stand for every possible instance of it at once; the reader can reinterpret any of the general solutions for any specific circuit polynomial that he/she needs—the permanental, characteristic, matching. (Moreover, some other B -polynomials can have the same properties, e.g., the

clique polynomial; see [20].) However, one would recognize that the most studied and widely used instance of the circuit polynomial is the *simple characteristic polynomial* $\phi^-(G; x)$ (see [33,6–13,25,26,30,17,21,18], where [6–8] (for chemists) are the world’s main monographs on the subject).

In order to proceed, we need to consider now some kinds of operations on graphs.

2.3. Some products of graphs

Let (G, u) and (H, v) be two graphs rooted at node u and v , respectively. We *attach* G to H (or H to G) by identifying node u of G with node v of H . Nodes u and v are called *nodes of attachment*. The node formed by identification is called the *coalescence node*. The resulting graph $G \circ H$ is called the *coalescence of G and H* .

Now consider a family $\{(U_1, u_1), (U_2, u_2), \dots, (U_t, u_t)\}$ of not necessary distinct graphs with roots u_1, u_2, \dots, u_t , respectively. We term a connected graph $U_1 \circ U_2 \circ \dots \circ U_t$ the *multiple coalescence of U_1, U_2, \dots, U_t* provided that nodes u_1, u_2, \dots, u_t are identified to reform the coalescence node r . We shall use $U^{|q|}$ to denote a q -fold coalescence of q isomorphic copies of a graph U ; in the same way, we shall use $G \circ H^{|s|}$ to denote the multiple coalescence of G and s copies of H , wherein all coalesced graphs have just one cutnode r in common, etc.

The above operation \circ is associative; in other words, it can be met as a generating operation in some semigroups of graphs. As a case in point, pick the set $\mathcal{U} = \{(U_j, u_j)\}_{j=1}^\infty$ of all unicomponental graphs; obviously, a pair $(\mathcal{U}; \circ)$ is an infinite commutative monoid of graphs, wherein the unity is represented by a one-vertex graph K_1 .

Let G be a graph with p nodes and $\Gamma = \{H_1, H_2, \dots, H_n\}$ a family of rooted graphs. Then the graph formed by attaching H_k to the k th ($1 \leq k \leq p$) node of G is called the *generalized rooted product* (see [20,28]) and is denoted by $G(\Gamma)$; G itself is called the *core of $G(\Gamma)$* . If each member of Γ is isomorphic to the rooted graph H , then the graph $G(\Gamma)$ is denoted by $G(H)$ [20,28,6,21]. Furthermore, if H is an edge (a twig), then the resulting graph is called a *thistle* or *equible graph* (see [20]).

Herein, we should make it our first business to treat some specific cases of the rooted product. Let a core G be a bipartite graph T , whose parts have p_1 and p_2 vertices, respectively; $p_1 \geq p_2$ and $p_1 + p_2 = p$. One can attach to every vertex in the first part of T an isomorphic copy of a graph H_1 and to every other vertex, in B , an isomorph of another graph H_2 ($H_1, H_2 \in \Gamma$); we shall locally call the resulting graph $T(\Gamma)$ the *restricted rooted product of graphs T and Γ* . It is worth specially noting an instance of it in which one type of graphs (either H_1 or H_2) is simply a one-vertex graph K_1 (with or without self-loops); that is, thus, in either part of T no attachment is made. Since the last case promises a nice operation for constructing more complex graphs of practical interest, we shall supply some relevant information about them.

An interesting generalization of the rooted product are the *F-graphs* [18], which are consecutively iterated rooted products defined as follows: $F^0 = K_1, F^1 = G, F^2 = G(H), \dots, F^{s+1} = F^s(H)$ ($s \geq 1$). Another interesting example of rooted product is the family of *dendrimers* D^k ($k \geq 0$) (see [14,15,20,28]), defined as follows: $D^0 = K_1, D^1 = G, D^2$ is the rooted product of G and H , in which some attachments of H are not made, i.e., H need not be attached to all nodes of G . In general, D^{s+1} ($s \geq 1$) is constructed from D^s ; and the number of copies attached to D^s obeys some fixed generation law. The dendrimers, in particular, imitate molecular structures, bearing the same name [22,1–4,32,14,15,20,28]. They are of practical significance [22,1–4,32]. This has lent impetus to the investigations in this paper as well.

A *monodendron* M is a maximal connected subgraph of a dendrimer D that shares only the coalescence node r with a core G ; in other words, it is a maximal (hyper)branch of D . Being a dendrimer in its own right, M has, however, two peculiarities. First, its core G is played by the same (weighted) graph H that is a structural repeating unit of branches ($G = H$). Second, a core G (or H) of M possesses the root (node r), which is not a feature of all dendrimers. Owing to its root r , the entire monodendron M can be made to serve the function of a new structural unit (instead of H) for constructing the higher dendrimers. Moreover, as well as any other dendrimer, M can serve as a hypercore in the same procedure, in lieu of a simple core $G = D^1$. As an instance of $\mathcal{D} = \{D^j\}_{j=0}^\infty$, the monodendron series $\mathcal{M} = \{M^j\}_{j=0}^\infty$ is defined as follows: $M^0 = K_1, M^1 = G = H$, and M^k ($k \geq 2$) is constructed by analogy with D^k above.

Let (a copy of) H invariably make $d + 1$ ($d < p(H)$) attachments inside a dendrimer D . Of this amount, 1 attachment is to hold the root of H itself while the other d are to hold the roots of all its incident neighbors in D . The number d is called a *progressive degree of H* (cf. [15]). A dendrimer is said to be *homogeneous* if all its monodendrons are equivalent and all prescribed attachments within it are made (cf. [15]). By definition, all dendrimers that we consider herein are homogeneous.

A monodendron M^j ($j \geq 1$) contains $1 + d + d^2 + \dots + d^{j-1} = (d^j - 1)/(d - 1)$ isomorphic copies of H therein; they are lying in concentric layers (tiers). This distribution correlates with their distance from a core G ; all copies of H that are built into one and the same tier are spaced at the same distance from G .

It is convenient to begin numbering the layers in a monodendron M from its core $G = H$ (thus receiving the ordinal 1). So, the number of layers in M^j ($j \geq 0$) equals j itself and the k th layer contains d^{k-1} isomorphic copies of H (and 0 under $k = 0$); the number of nodes, in the j th (outermost) layer, that can be used for further attachments is d^j .

We come now to an important remark. The matter is that the above procedure that successively generates all monodendrons M^j of a series \mathcal{M} is unambiguous; it always reproduces one and the same monodendron M^j with a given number j of tiers. So, it is impossible to produce instead of M^j any other homogeneous monodendron with j layers. Hence it follows that the number $j \geq 0$ of layers uniquely characterizes a homogeneous monodendron M^j in a specific series \mathcal{M} .

In a general way, a monodendron M^j and d^j isomorphic copies of a monodendron M^k ($j, k \geq 0$), when used as G and H , respectively, afford a monodendron M^{j+k} (see above). We shall use the notation $M^j \star M^k = M^{j+k}$ to denote this. The binary operation \star is obviously commutative and associative: $M^j \star M^k = M^k \star M^j$ and $M^j \star (M^k \star M^l) = (M^j \star M^k) \star M^l$ ($j, k, l \geq 0$), which can readily be verified, recalling that the number of tiers in the resulting monodendron uniquely characterizes it. Since $M^0 = K_1$ acts as the identity, we can at once conclude that $(\mathcal{M}; \star)$ is an infinite commutative monoid isomorphic to the additive monoid $(\mathbb{N}; +)$ of all nonnegative integers. One can simply say that \mathcal{M} is a monoid (without indicating its operation) and also adopt the multiplicative notation $M^j M^k$ for $M^j \star M^k$ and in any similar case. The said \mathcal{M} herein resembles two earlier-studied situations [18,31] (see [27]) in every essential detail.

Now we need to consider some known results that will be used below.

2.4. Basic results

We begin with a previous result (see [20, Lemma 5]), rewritten here as follows:

Lemma 1. *Let $G \circ H$ be the graph formed by attaching a graph G to a graph H , and let r be the resulting coalescence node. Then*

$$B(G \circ H; \mathbf{x}; \mathbf{w}) = B(H_{-r}; \mathbf{x}; \mathbf{w}) [B(G; \mathbf{x}; \mathbf{w})]_{x_r \rightarrow B(H^\Delta; \mathbf{x}; \mathbf{w})/B(H_{-r}; \mathbf{x}; \mathbf{w})}, \tag{10}$$

where H_{-r} is a graph H less its root r , and H^Δ is the graph H less its self-loops lying in the vertex r .

An important result is the following statement (see [20, Theorem 2]):

Theorem 2. *Let G be a graph with p vertices and $\Gamma = \{H_1, H_2, \dots, H_p\}$ be a family of rooted graphs. Then*

$$B(G(\Gamma); \mathbf{x}; \mathbf{w}) = \left[\prod_{i=1}^p B(L_i; \mathbf{x}; \mathbf{w}) \right] [B(G; \mathbf{x}; \mathbf{w})]_{x_i \rightarrow B(H^\Delta; \mathbf{x}; \mathbf{w})/B(L_i; \mathbf{x}; \mathbf{w})} \quad (1 \leq i \leq p), \tag{11}$$

where L_i ($1 \leq i \leq p$) is the graph H_i with its root removed (i.e., $H_i - r_i$), and H_i^Δ is the graph H_i with all the self-loops at the root removed.

In the case of the simple rooted product, one can derive the following corollary of Theorem 2 for the simple B -polynomial (see [20, Corollary 2.1]), viz.:

Corollary 2.1. *Let G and H be rooted graphs. Let $G(H)$ be the graph obtained by attaching an isomorph of H to each of the p nodes of G . Then*

$$B(G(H); x) = [B(H_{-r}; x)]^p [B(G; x)]_{x \rightarrow B(H^\Delta; x)/B(H_{-r}; x)}, \tag{12}$$

where H^Δ is the graph H with all loops at its root r removed.

Here, we should note earlier specific versions of Lemma 2 for the characteristic [21,6] and matching [6] polynomials (wherein only unweighted graphs have been treated).

Now recall that any simple B -polynomial, such as $B(G; x)$ in (11), can be expanded in powers of x ; therefore, we can write down it as

$$B(G; x) = \gamma_0 x^p + \gamma_1 x^{p-1} + \dots + \gamma_p x^0 \quad (\gamma_0 = 1). \tag{13}$$

Owing to (13), we can give herein a new version of Lemma 3 from [28], viz.:

Lemma 3. *Let G and H be rooted graphs. Let $G(H)$ be the rooted product of G and H , as above. Then*

$$B(G(H); x) = \sum_{g=0}^p \gamma_g [B(H^\Delta; x)]^{p-g} [B(H_{-r}; x)]^g, \tag{14}$$

where H^Δ is the same as above.

The next quotation [20, Corollary 2.2]) appears herein as follows:

Lemma 4. *Let G and H be rooted graphs. Let $G(H)$ be the graph obtained by attaching an isomorph of H to each of the p nodes of G . Also, let $\lambda_1, \lambda_2, \dots, \lambda_p$ be the roots of $B(G, x)$. Then*

$$B(G(H); x) = \prod_{i=1}^p [B(H^\Delta; x) - \lambda_i B(H_{-r}; x)]. \tag{15}$$

Notice that H^Δ is misprinted in the original text [20, Corollary 2.2] as H .

We can also derive a special corollary (see [20, Corollary 2.3]) from Lemma 4, viz.:

Lemma 5. *Let 0 be a k -fold ($k \geq 1$) root of $B(G; x)$. Then $[B(H^\Delta; x)]^k$ divides $B(G(H); x)$.*

Here, we cannot help stating another lemma (see [28, Lemma 6]) that generalizes Lemmas 4 and 5. First, denote by H_{λ_i} ($1 \leq i \leq p$) the graph obtained by attaching a self-loop with the weight $b_r = -\lambda_i$ to node r of H^Δ . It is not difficult to establish that the expression in square brackets, in (15), is just $B(H_{\lambda_i}; x)$, which immediately affords us a derived result, viz.:

Lemma 6. *Let G and H be rooted graphs. Let $G(H)$ be the graph obtained by attaching an isomorph of H to each of the nodes of G . Also, let H_{λ_i} ($1 \leq i \leq p$) be defined as above. Then*

$$B(G(H); x) = \prod_{i=1}^p B(H_{\lambda_i}; x). \tag{16}$$

One additional definition that will be employed below is this. Let $m_1(\lambda)$ and $m_2(\lambda)$ be the multiplicities of a specific root λ for polynomials $B(G_1; x)$ and $B(G_2; x)$, respectively. We shall call the number $m(\lambda) = \min(m_1(\lambda), m_2(\lambda))$ a *common multiplicity of an eigenvalue λ* for the polynomials $B(G_1; x)$ and $B(G_2; x)$.

Now we shall turn to deriving new results.

3. Main results

Our first result will be complementary to Theorem 2:

Theorem 7. *Let G be a graph with p vertices and $\Gamma = \{H_1, H_2, \dots, H_p\}$ be a family of rooted graphs. Then*

$$B(G(\Gamma); \mathbf{x}; \mathbf{w}) = \left[\prod_{i=1}^p B(L_i; \mathbf{x}; \mathbf{w}) \right] [B(G^\square; \mathbf{x}; \mathbf{w})]_{x_i \rightarrow B(H_i; \mathbf{x}; \mathbf{w})/B(L_i; \mathbf{x}; \mathbf{w})} \quad (1 \leq i \leq p). \tag{17}$$

Proof. Sketch it. Since the graphs G and H play a symmetrical role in Lemma 1, one can rewrite (10) in an equivalent form as follows:

$$B(G \circ H; \mathbf{x}; \mathbf{w}) = B(G_{-r}; \mathbf{x}; \mathbf{w})[B(H; \mathbf{x}; \mathbf{w})]_{x_i \rightarrow B(G^\Delta; \mathbf{x}; \mathbf{w})/B(G_{-r}; \mathbf{x}; \mathbf{w})} \quad (1 \leq i \leq p). \tag{18}$$

Recall that Theorem 2 was proven in [20] by repetitively applying Lemma 1 to $G(\Gamma)$. If we now use p times (18) instead of (10), we arrive at the result, wherein self-loops are (gradually) removed from the core G rather than from the root r_i of every graph H_i (in contrast to theorem 2). Therefore, denoting by G^\square the core G less all its self-loops (which is thus obtained), we arrive at (17). \square

Herein, we are interested in deriving a few corollaries of Theorem 7. First, we shall state the following mate of Corollary 2.1:

Corollary 7.1. *Let T be a bipartite graph with the bipartition into p_1 and p_2 vertices, accordingly ($p_1 \geq p_2$; $p_1 + p_2 = p$). Let further $T(\Gamma)$ be the restricted rooted product of graphs T and Γ , wherein an isomorphic copy of a graph H_1 is attached to every vertex of the first part of T and an isomorph of another graph H_2 is attached to every vertex of the second part of T ($H_1, H_2 \in \Gamma$). Then*

$$B(T(\Gamma); x) = [P(L_1; x)]^{p_1}[P(L_2; x)]^{p_2}[P(T^\square; y_1, y_2)]_{y_i \rightarrow P(H_i; x)/P(L_i; x)} \quad (i = 1, 2), \tag{19}$$

where T^\square is the graph T less all its self-loops, and y_i ($i = 1, 2$) simultaneously stands for all indexed x -variables belonging to the vertices of the i th part of T .

As an initial prerequisite to the next corollary, one can return to (13). It gives an idea to expand $P(T^\square; y_1, y_2)$ of (19) as follows:

$$P(T^\square; y_1, y_2) = \delta_0 y_1^{p_1} y_2^{p_2} + \dots + \delta_k y_1^{p_1-k} y_2^{p_2-k} + \dots + \delta_{p_2} y_1^{p_1-p_2} y_2^0 \quad (\delta_0 = 1; p_1 \geq p_2), \tag{20}$$

where the adjunct powers of y_1 and y_2 decrease synchronously. The matter is that all the F -covers (see (1)) that correspond to the circuit polynomial $P(T^\square; y_1, y_2)$ of a bipartite loopless graph T^\square should consist just of cycles of even length (since only such cycles are in it). Evidently, every F -cover always covers one and the same number k ($1 \leq k \leq p$) of vertices pertaining to both parts of T^\square (i.e., k green vertices and k red ones). Hence, it immediately follows the above property of the powers in (20). The obtained expansion affords the following corollary, of Theorem 7, accompanying Lemma 3:

Lemma 8. *Let $P(T(\Gamma); x)$ be the circuit polynomial of the restricted rooted product $T(\Gamma)$ as above. Then*

$$P(T(\Gamma); x) = \sum_{k=0}^{p_2} \delta_k [P(H_1; x)]^{p_1-k} [P(H_2; x)]^{p_2-k} [P(L_1; x)]^k [P(L_2; x)]^k \quad (p_1 \geq p_2). \tag{21}$$

As it was already discussed in the Preliminaries, of our special interest are instances $T(H)_1$ and $T(H)_2$ of $T(\Gamma)$ in which isomorphic copies of an arbitrary graph H are attached just to the vertices of either part of T (while no attachment whatever is done to the other part of it). This affords two complementary corollaries of Lemma 8.

Corollary 8.1. *Let $T(H)_1$ be the restricted rooted product of a bipartite graph T and an arbitrary graph H in which an isomorphic copy of H is attached just to every vertex of the first (greater) part of T . Then*

$$P(T(H)_1; x) = \sum_{k=0}^{p_2} \delta_k (x + b_2)^{p_2-k} [P(H; x)]^{p_1-k} [P(H_{-r}; x)]^k \quad (p_1 \geq p_2), \tag{22}$$

where b_2 is a common total weight of self-loops lying in each vertex of the second (smaller) part of T .

Corollary 8.2. *Let $T(H)_2$ be the restricted rooted product of a bipartite graph T and an arbitrary graph H in which an isomorphic copy of H is attached just to every vertex of the second (smaller) part of T . Then*

$$P(T(H)_1; x) = \sum_{k=0}^{p_2} \delta_k (x + b_1)^{p_1-k} [P(H; x)]^{p_2-k} [P(H_{-r}; x)]^k \quad (p_1 \geq p_2), \tag{23}$$

where b_1 is a common total weight of self-loops lying in each vertex of the first (greater) part of T .

Now we recall that any circuit polynomial $P(T^\square; x)$ of a bipartite graph T^\square without self-loops necessarily has at least $(p_1 - p_2)$ zero eigenvalues (or roots), and together with every of its eigenvalue μ it also possesses an eigenvalue $-\mu$ (in particular see [7, Theorem 3.11]). In order to demonstrate this, one can substitute x for y_1 and y_2 on the RHS of (20), which gives

$$P(T^\square; x) = \delta_0 x^p + \delta_1 x^{p-2} + \dots + \delta_{p_2} x^{p_1-p_2} \quad (p_1 \geq p_2; p = p_1 + p_2). \tag{24}$$

It is immediately seen that $P(T^\square; x)$ is divisible by $x^{p_1-p_2}$ and, therefore, possesses at least $(p_1 - p_2)$ zero eigenvalues. Further, all the powers of x on the RHS of (24) have one and the same parity (either even or odd); and thereby the negative $-\mu$ of every root μ of $P(T^\square; x)$ is also a root of it. By this reason, we shall consider below only squares of the roots, which, excluding necessary $(p_1 - p_2)$ 0's, will comprise exactly p_2 ($p_2 \leq p_1$) not necessarily distinct numbers: $\mu_1^2, \mu_2^2, \dots, \mu_{p_2}^2$ (whose order does not matter). This allows us to rewrite (24) as follows:

$$P(T^\square; x) = x^{p_1-p_2} \prod_{i=1}^{p_2} (x^2 - \mu_i^2) \quad (p_1 \geq p_2). \tag{25}$$

Here, recall that, by definition, γ_k is simultaneously the coefficient of x^{p-k} on the RHS of (24) and of $y_1^{p_1-k} y_2^{p_2-k}$ on the RHS of (20); $1 \leq k \leq p_2 \leq p_1$; $p_1 + p_2$. Among other things, this assures the reverse passage from (24) to (20). But the RHS of (24) is equal to the RHS of (25); therefore, we can legitimately rewrite (25) in two variables, y_1 and y_2 , as well:

$$P(T^\square; y_1, y_2) = y_1^{p_1-p_2} \prod_{i=1}^{p_2} (y_1 y_2 - \mu_i^2) \quad (p_1 \geq p_2). \tag{26}$$

In the present paper, (26) is an important requisite because it enables us to state the following crucial sentence resembling Lemma 4:

Lemma 9. *Let $P(T(\Gamma); x)$ be the circuit polynomial of the restricted rooted product $T(\Gamma)$ of graphs T and Γ (see above). Then*

$$P(T(\Gamma); x) = [P(H_1; x)]^{p_1-p_2} \prod_{i=1}^{p_2} [P(H_1; x)P(H_2; x) - \mu_i^2 P(L_1; x)P(L_2; x)] \quad (p_1 \geq p_2). \tag{27}$$

Proof. Taking into account the definition of collective variables y_1 and y_2 (instead of respective x_i 's in (17)) and expressing $P(T^\square; \mathbf{x}; \mathbf{w})$ in a specific form of the RHS of (26), we can easily conclude that this statement is simply a corollary of Theorem 7. Hence, the proof is immediate. \square

Note that interchanging the sorts of graphs H_1 and H_2 in $T(\Gamma)$ (together with the weights b_1 and b_2) results in another product $T(\Gamma)'$, which can be called, in the chemical language, a *substitutional isomer* of $T(\Gamma)$. Under $p_1 = p_2$, the two substitutional isomers $T(\Gamma)$ and $T(\Gamma)'$ are distinguished only by the reciprocal fashion in which the rooted graphs of sorts H_1 and H_2 are attached to the core T in them. Therefore, we shall call the last pair of substitutional isomers *reciprocal rooted products*. This leads to the following corollary:

Corollary 9.1. *Let T be an equipartite bipartite graph ($p_1 = p_2$) and let $T(\Gamma)$ and $T(\Gamma)'$ be the reciprocal (restricted) rooted products. Then*

$$P(T(\Gamma); x) = P(T(\Gamma)'; x). \tag{28}$$

Proof. Indeed, under $p_1 = p_2$, the indices 1 and 2 play symmetrical roles on the RHS of (27); consequently, the interchanging of these indices cannot alter the result. Hence, the proof is immediate. \square

Here, the chemical reader may guess that heteroatoms in a molecule can be treated in much the same manner as distinct chemical substituents above. Or, in mathematical terms, a bipartite graph T may possess green vertices with the weight b_1 and red ones with the weight b_2 ; interchanging b_1 and b_2 is just tantamount to the passage to the reciprocal product (which is here simply a reweighted graph T , wherein no (re-)attachments of any graphs H_1 and H_2 are made).

In a philosophical sense, it is very interesting that there exist nonisomorphic graphs for which every specific circuit polynomial (characteristic, permanent, matching) should be equal. Here, we recall that two graphs G_1 and G_2 are called *isospectral* (or *cospectral*) (see [7]) if $P(G_1; x) = P(G_2; x)$; under this, the type of the polynomial P specifically depends on the context. Studying isospectral graphs is an important aspect of the theory of graph [7] and its application (see [8]).

Regrettably, only in a descriptive form, the author dares to propose the simplest example of isospectral reciprocal products. First of all, note that under $p_1 = p_2$ the minimal bipartite graph in which the parts are not equivalent (on interchanging the colors of their vertices) is a tree with six vertices. That tree is represented by a simple path spanning five vertices, with the sixth vertex located at a free end of the edge attached to the third (middle) vertex of it (see the tree 2.12 in [7, Table 2]). The chemical reader at once recognizes, in this tree, a hydrogen-depleted graph of the carbon skeleton of 3-methyl- n -pentane (where hydrogen atoms are not taken into account). We assume that the green vertices are located on the longest five-vertex chain of this tree at sites 1, 3, and 5 while the red vertices are at sites 2, 4, and at the end of the twig. Attaching an isomorph copy of an arbitrary graph H_1 (which represents a chemical radical) to the green vertices and an isomorph of another graph H_2 to the red vertices produces the product $T(\Gamma)$. The same process performed in a reciprocal fashion (when sorts of graphs H_1 and H_2 are interchanged) does the reciprocal rooted product $T(\Gamma)'$. Under this, the two restricted rooted products are always isospectral; that is, the graphs $T(\Gamma)$ and $T(\Gamma)'$ should necessarily have one and the same circuit polynomial. Further, let H_1 be a one-vertex graph K_1 (that is, no attachments should be made to the respective sites) and H_2 be a two-vertex complete graph K_2 (i.e., an edge, or a twig). Then, $T(\Gamma)$ (or the tree 2.74 [7, Table 2]) is a hydrogen-depleted graph of 2,4-dimethyl-3-ethyl- n -pentane while $T(\Gamma)'$ (or the tree 2.75 in [7, Table 2]) is a hydrogen-depleted graph of 4,4'-dimethyl- n -heptane. As it follows from Table 2 of the cited book, both of (molecular) graphs have the same characteristic polynomial (of the adjacency matrix), viz.:

$$P(T(\Gamma); x) = P(T(\Gamma)'; x) = x^9 - 8x^7 + 18x^5 - 12x^3,$$

with the roots (eigenvalues): $\lambda_1=2.175$; $\lambda_2=1.414$; $\lambda_3=1.126$; $\lambda_4=\lambda_5=\lambda_6=0$; $\lambda_7=-1.126$; $\lambda_8=-1.414$; $\lambda_9=-2.175$. Possibly, [7] enables the reader to find other instances of such graphs.

Now recall the definition of the restricted rooted products $T(H)_1$ and $T(H)_2$, used in Corollaries 8.1 and 8.2, respectively. We can derive similar corollaries of Lemma 9 as well:

Corollary 9.2. Let $P(T(H)_1; x)$ be the circuit polynomial of the restricted rooted product $T(H)_1$. Then

$$P(T(H)_1; x) = [P(H; x)]^{p_1 - p_2} \prod_{i=1}^{p_2} [(x + b_2)P(H; x) - \mu_i^2 P(H_{-r}; x)], \quad (29)$$

where b_2 is the weight of every vertex of the second (smaller) part of T .

Corollary 9.3. Let $P(T(H)_2; x)$ be the circuit polynomial of the restricted rooted product $T(H)_2$. Then

$$P(T(H)_2; x) = (x + b_1)^{p_1 - p_2} \prod_{i=1}^{p_2} [(x + b_1)P(H; x) - \mu_i^2 P(H_{-r}; x)], \quad (30)$$

where b_1 is the weight of every vertex of the first (greater) part of T .

Here, we remind that the weight b_i ($i \leq p$) of the i th vertex is a total weight of all self-loops lying in this vertex. Lemma 9 and Corollaries 9.2 and 9.3 resemble Lemma 4. This list of comparisons can be continued.

Corollary 9.4. *Let 0 be an s -fold ($s \geq p_1 - p_2$) root of the circuit polynomial $P(T(\Gamma); x)$ of the restricted rooted product $T(\Gamma)$. Then $[P(H_1; x)]^s [P(H_2; x)]^{s-p_1+p_2}$ divides $P(T(\Gamma); x)$.*

What roots μ are inherited by $(T(\Gamma); x)$ from the polynomials $P(H_1; x)$, $P(H_2; x)$, $P(L_1; x)$, and $P(L_2; x)$, involved in the above formulae, also depends on a common multiplicity $m(\mu)$ of every root μ for four independent pairs $(P(H_i; x); P(L_j; x))$ ($i, j \in \{1, 2\}$) of these polynomials. Obviously, if $m(\mu) \geq 1$ in at least one of the four cases the respective root μ is also inherited by $P(T(\Gamma); x)$ (with the multiplicity not less than $m(\mu)$). If $m(\mu) = 0$ for all the four variants, it (still) remains to employ Corollary 9.4, which works in a complementary manner to the common-multiplicity principle. A more detailed investigation is left here to the reader. However, we want to make yet some qualitative remarks, addressed chiefly to the chemical audience. First, the degeneracy of the roots of $P(T^\square; x)$ is beneficial for the multiplicity of the roots of $P(T(\Gamma); x)$. Second, as well known, the root $\mu = 0$ of the characteristic polynomial of a molecular graph is unfavorable for the stability of the molecule which is represented by it (see [8,7]). Nevertheless, the construction of the restricted rooted product can harvest the same (or even more) benefits from the zero eigenvalue. That is why the materials engineer must not a priori rule out the core graphs T^\square with the eigenvalue(s) $\mu = 0$.

Now note that the factor $[P(H_1; x)P(H_2; x) - \mu_i^2 P(L_1; x)P(L_2; x)]$ involved on the RHS of (27) is, in its own right, the circuit polynomial $P(H_{\mu_i^2}; x)$ of some derivative graph $H_{\mu_i^2}$. Here, the graph $H_{\mu_i^2}$ is obtained by joining with the edge $r_1 r_2$ of the weight μ_i^2 the roots r_1 and r_2 of graphs H_1 and H_2 , respectively; see the necessary general theory in [28,7]. Under this, it is worth recalling that the weight μ_i^2 of the edge $r_1 r_2$ is, by definition, the product $a'_{r_1 r_2} a'_{r_2 r_1}$ of the entries $a'_{r_1 r_2}$ and $a'_{r_2 r_1}$ of the adjacency matrix A' of the graph $H_{\mu_i^2}$. Our done preparation allows us to rewrite Lemma 9 in the following equivalent form:

Lemma 10. *Let $P(T(\Gamma); x)$ be the circuit polynomial of the restricted rooted product $T(\Gamma)$ of graphs T and Γ . Then*

$$P(T(\Gamma); x) = [P(H_1; x)]^{p_1-p_2} \prod_{i=1}^{p_2} P(H_{\mu_i^2}; x) \quad (p_1 \geq p_2), \tag{31}$$

where $P(H_{\mu_i^2}; x)$ is defined as above.

Lemma 10, derived for the circuit polynomial of the restricted rooted product $T(\Gamma)$, resembles Lemma 6 for the B -polynomial of the unrestricted rooted product $G(H)$ (see [20,28]). Moreover, we notice in passing that all the results above that involve the bipartite core graph T^\square also hold good for the clique polynomial of $T(\Gamma)$ (see [20]).

Seeing the RHS of (31), one can immediately conclude that there exists such a similarity transformation of the adjacency matrix $A(T(\Gamma))$ of the restricted rooted product $T(\Gamma)$ that block-diagonalizes it (to the form which is consistent with the RHS of (31)). The sense of the said can be better evaluated if one recalls how difficult it is, in general, to find whatever similarity transformation simultaneously conserving all types of the circuit polynomial (of an arbitrary matrix); usually, it is possible only for the characteristic polynomial while renders impossible for the permanent and/or matching polynomial.

4. Discussion

1. By virtue of the results obtained herein, the circuit polynomial $P(T(\Gamma); x)$ of the restricted rooted product $T(\Gamma)$ can uniquely be reconstructed from the collection of circuit polynomials $P(T^\square; x)$, $P(H_1; x)$, $P(H_2; x)$, $P(L_1; x)$, and $P(L_2; x)$ of graphs T^\square , H_1 , H_2 , L_1 , and L_2 , consecutively. This seems to be of use because, otherwise, it would be very difficult to estimate the spectrum (of eigenvalues) of a complex target graph $T(\Gamma)$ (res. molecule), as is necessarily for creating substances with given electronic and photonic properties.

2. Degenerate roots of the circuit polynomial $P(T(\Gamma); x)$ play an important role, in the present context. The degeneracy of eigenvalues, first of all, tautologically means the possibility of filling some (needed) energy levels, in a molecule or bulk material, to a rather higher degree than it takes place for undegenerated eigenvalues. The said is profitable not only for electronic and photonic properties (of substances), as such, but can well be addressed to treating diverse surfaces or substrates in order to passivate these or, on the contrary, make more catalytically active, hydrophilic, etc.

Under this, in particular, a surface can acquire the properties of a chemical group represented by a graph H_1 in cases when the latter multiply contributes to the resulting spectrum of the system represented by the graph $T(I)$ (see [28]).

3. A prospective trend, which is yet beyond the present scope, is engineering dendrimers (both graphs and molecules) that iteratively uses the construction of the restricted rooted product $T(I)$. This can essentially extend the capabilities of previous approaches (see [28]). Here, it is especially worth merging the methods of such work as [28] with those obtained herein.

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