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The Block–Polynomials and Block–Spectra of Dendrimers

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The Block–Polynomials and Block–Spectra of Dendrimers[#]

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Abstract

Motivation. Dendrimers represent a novel class of hyperbranched supramolecular structures, that promoted novel fundamental and applicative research. Applications of dendrimers include simulation of enzymatic reactions, artificial vaccines, gene carriers and homogeneous catalysis. The polynomial description of molecular structures is one of the most essential and elegant procedure of encoding topological properties and providing valuable descriptors, such as polynomial roots and coefficients.

Method. From the mathematical point of view, dendrimers represent a generalized recursive class of graphs. The block construction of dendrimers is simulated with block polynomials, which allow the study of their roots, *i.e.*, their spectrum of eigenvalues.

Results. The study of the block polynomial behavior envisaged the transmittance of hereditary spectral properties along a recursive series of dendrimers.

Conclusions. A novel description of supramolecular dendritic molecules is given. The obtained results can be used to design molecular structures with tailored electronic and photonic properties.

Keywords. Block polynomials; spectrum of eigenvalues; hereditary properties; dendrimers.

Abbreviations and notations

A–polynomial, articulation node polynomial
B–polynomial, block polynomial
F–polynomial, Farrell's polynomial

1 INTRODUCTION

Recent years have witnessed a dramatic growth of interdisciplinary research activity involving materials that exhibit special electronic and photonic properties. Increasing interest has been shown in a new type of oligomeric molecular architectures that are called dendrimers [1–6]. These three–dimensional globular structures possessing a cactus–like skeleton have found practical use in many areas [1–6], including modern electronics [3–6].

Graphically, the molecular dendrimers generalize the arborescent patterns that are known for regular branching processes. Currently, the practical results suggest intensive graph–theoretical

[#] Dedicated on the occasion of the 70th birthday to Professor Alexandru T. Balaban.
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studies of the generalized recursive class of dendritic graphs bearing the same collective name [7–9]. This paper continues the study of the common spectral features of these graphs, from our previous work [9].

The block polynomial $B(G;x)$ of a graph G (or the B–polynomial, for short) was introduced by Farrell and Rosenfeld [9] in the study of spectral properties of graphs with articulation points (in particular, dendrimers). The B–spectrum of the eigenvalues of G is a collection of all the roots of an individual B–polynomial $B(G;x)$. An intriguing area of investigation is the transmittance of hereditary spectral properties [9] along a recursive dendrimer series, wherein each next dendrimer inherits some or all eigenvalues of its predecessors. In particular, this trend seems to be valuable in electronics [3–6]. In order to satisfy the needs of the experimentalist, one has to take into account the general case of arbitrary weighted digraphs which is necessary for correctly finding the energy levels of dendritic matter.

A further mathematical direction may be investigation of all possible types of graph polynomials of dendrimers (and respective spectra thereof), which eventually can be useful in predicting thermodynamic properties of dendritic materials [10–11]. The literature on graph polynomials is quite extensive [9,12–17] and papers like [13] are of great importance in this context. Rigorous theorems about dendrimers may underlie the theoretical basis for calculating all the above polynomials while contacts with the nonmathematical researcher, if any, supplement analytical findings with interesting applications as well [18–22,25].

2 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 by Farrell [12]. 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*** a weight w_α. The weight of a cover ***G*** denoted by $w(G)$, is the product of the weights of its components. Then the F–polynomial is

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

where the summation is taken over all the ***F***–covers of G, and **w** is a vector of the weights 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 $x_i + b_i$ $(1 \le i \le p)$, where x_i is an indeterminate and b_i is the sum of weights of all loops, if any, lying on a vertex i [16,17]. 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 l'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 F–polynomial of G.

If every non–node 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. Note that if we take F to be a family of cycles, then every non–node 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 [9] are examples of block polynomials. We therefore classify all the special circuit polynomials, for example the matching, characteristic and permanental polynomials [9,14–23] as B–polynomials.

Observe that the families that give rise to B–polynomials consist of graphs characterized by the number of vertices. Therefore, when general weights are assigned to the members of F, it is sufficient to associate to each member of F (having n vertices) the weight w_n. The resulting B–polynomial would therefore contain monomials that totally describe the covers. In this general F–polynomial, the vector of weights is $\mathbf{w} = (w_1, w_2, \ldots, w_p)$. Note that if F is the family of stars or paths the number of nodes characterizes every member of F. 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 other 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 acyclic polynomial, which was defined independently [9]. The same matching polynomial yields, under certain substitutions, the chromatic polynomial for certain classes of graphs and a whole group of its relatives [9]. The classical rook polynomial [9] is yet another relative of the matching polynomial.

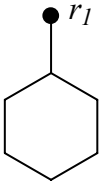
Note that the most general F–polynomial is the subgraph polynomial [9], since it enables us to derive, in principle, any other F–polynomial. However, the subgraph polynomial is not a B–polynomial. There exist other classes of F–polynomials of interest, e.g., the articulation node polynomials or A–polynomials [9]. At this point, we need to consider some kinds of operations on graphs.

3 SOME PRODUCTS OF GRAPHS

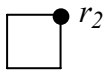
Let (G, u) and (H, v) be two graphs rooted at node u and v, respectively. We attach G to H (or H to G) by identifying node u of G with node v of H. Nodes u and v are called nodes of attachment. The node formed by identification is called the coalescence node. The resulting graph $G\ o\ H$ is called the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

Now consider a family $\{(U_1, u_1), (U_2, u_2), \ldots, (U_t, u_t)\}$ of not necessary distinct graphs with roots $u_1, u_2, \ldots, u_t$, respectively. We term a connected graph U_1 o U_2 o … o U_t the multiple coalescence

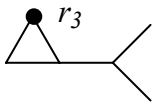
of U_1, U_2, ..., U_t provided that nodes u_1, u_2, …, u_t are identified to reform the coalescence node r. We shall use $\boldsymbol{U}^{|q|}$ to denote a q–uple coalescence of q isomorphic copies of a graph U; in the same way, we shall use $\boldsymbol{G}\ o\ \boldsymbol{H}^{|s|}$ to denote the multiple coalescence of G and s copies of H, wherein all coalesced graphs have just one cut node r in common. Some graphs and their operations will herein be illustrated.



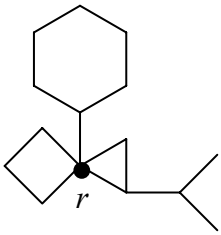
$U = U_1$



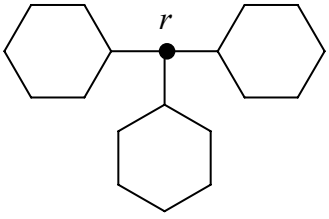
$G = U_2$



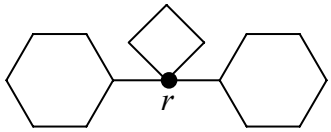
$H = U_3$



U_1 o U_2 o U_3

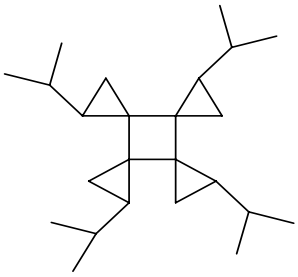


$U^{|3|}$

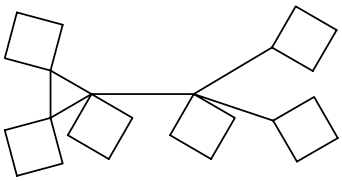


G o $U^{|2|}$

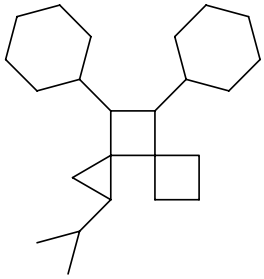
The above operation o is associative; in other words, it can be met as a generating operation in some semigroups of graphs. As a case in point, pick the set $\boldsymbol{U} = \{U_j)\}_{j=1}^{\infty}$ of all unicomponental graphs; obviously, a pair ($\boldsymbol{U}$; o) is an infinite commutative monoid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



$G(H)$

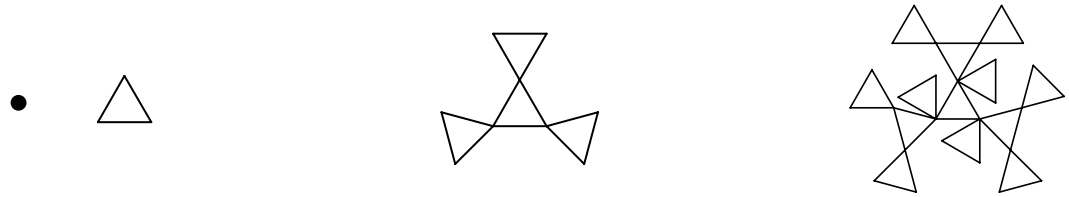


$H(G)$



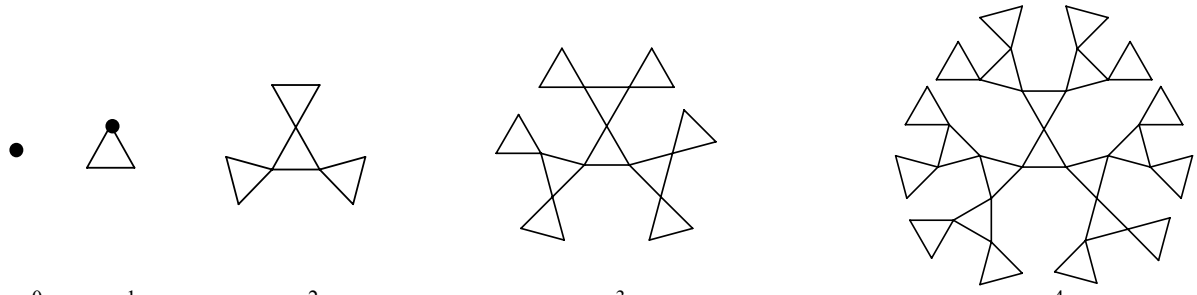
$G\ (\Gamma)$; $\Gamma = \{U_1, U_1, U_2, U_3\}$

Let G be a graph, consisting of n nodes and $\Gamma = \{H_1, H_2, \ldots, H_n\}$ a family of rooted graphs. Then the graph formed by attaching H_k to the k–th ($1 \le k \le p$) node of G is called the generalized rooted product [9] 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 $G(H)$ [15,23]. Furthermore, if H is a wedge (a twig), then the resulting graph is called a thistle or equible graph [9]. An interesting generalization of the rooted product are the F–graphs [13], which are consecutively iterated rooted products defined as: $F^0 = K_1$, $F^1 = G$, $F^2 = G(H)$, ..., $F^{s+1} = F^s(H)$, $s \ge 1$.



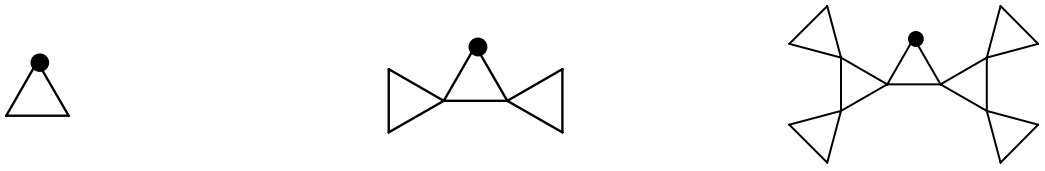
F^0 F^1 F^2 F^3

A family of dendrimers D^k ($k \geq 0$) is just a rooted product [9] defined as: $D^0 = K_1$, $D^1 = G$, 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 [1–9]. Their practical importance [1–6] is the motivation for investigations reported in this paper.



D^0 D^1 D^2 D^3 D^4

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 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, instead of a simple core $G = D^1$. As an instance of $\boldsymbol{D} = \{D^j)\}_{j=0}^{\infty}$, the monodendron series $M = \{M^j)\}_{j=0}^{\infty}$ is defined as $M^0 = K_1$, $M^1 = G = H$ and M^k ($k \geq 2$) is constructed by analogy to D^k (see above).



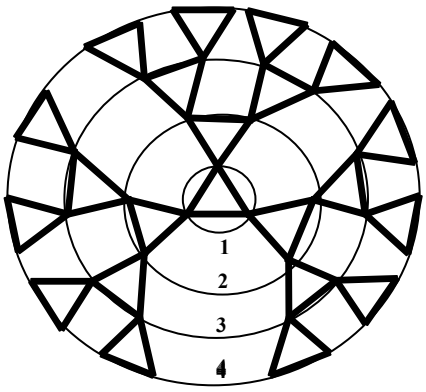
M^1 M^2 M^3

Let (a copy of) H invariably make $d + 1$, with $d < p(H)$, attachments inside a dendrimer D. Of

this amount, 1 attachment holds for 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* [8]. A dendrimer is said homogeneous if all its monodendrons are equivalent and all prescribed attachments within it are made [8]. By definition, all dendrimers that we consider herein are homogeneous.

A monodendron M^j ($j \geq 1$) contains $1 + d + d^2 + ... + d^{j-1} = (d^j - 1) / (d - 1)$ 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*.

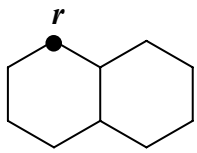
It is convenient to begin numbering the layers in a monodendron *M* from its core $G = H$ (thus receiving the ordinal 1). So, the number of layers in M^j ($j \geq 0$) equals to *j* itself and the *k*–th layer contains d^{k-1} isomorphic copies of *H* (and 0 under $k = 0$); the number of nodes, in the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



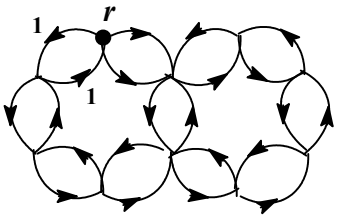
We come now to an important remark: the above procedure, successively generating all monodendrons M^j of a series *M*, is unambiguous. It always reproduces one and the same monodendron M^j with a given number *j* of tiers. So, it is impossible to produce, out of M^j, any other homogeneous monodendron 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 *M*.

In general, a monodendron M^j and d^j isomorphic copies of the monodendron M^j (used as *G* and *H*, respectively) afford a monodendron M^{j+k} ($j, k \geq 0$, see above). We can write this as: $M^j * M^k = M^{j+k}$. The binary operation * is obviously commutative and associative: $M^j * M^k = M^k * M^j$ and $M^j * (M^k * M^l) = (M^j * M^k) * M^l$ ($j, k, l \geq 0$), which can easily 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 (M;*) is an infinite commutative monoid isomorphic to the additive monoid (N; +) of all nonnegative integers. One can simply say that *M* is a monoid (without indicating its operation) and adopt the multiplicative notation $M^j M^k$ for $M^j * M^k$. The *M* herein discussed resembles two earlier–studied situations [13,24] in every essential detail.

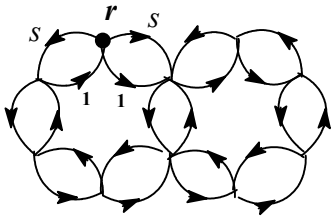
In order to proceed, we need some preparations. Let U be an arbitrary connected (weighted) graph with the root r. In the context of the B–polynomials (see above), U can be characterized by a family F of its connected (weighted) subgraphs, which are strictly selected for each specific sort of the B–polynomials [9,12–17]. Regardless of a sort of the B–polynomial, one can distribute the whole family F into two parts F_1 and F_2, where F_1 stands for subgraphs of F covering the node r and F_2 does for the remaining subgraphs of F. Given an arbitrary fixed natural s, substitute the weight $sw(\alpha)$ for the original weight $w(\alpha)$ of every subgraph $\alpha \in F_1$ and denote by S the newly–weighted graph thus obtained (where S is reminiscent of s). Evidently, graphs U and S are isomorphic and possess identical roots.



U



U

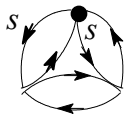


S

We shall also need in a generalized analog T of the graph S. The graph T is defined through the same reweighting $w(\alpha) \rightarrow sw(\alpha)$ from the coalescence $G\ o\ U$ provided that reweighted therein are only subgraphs $\alpha \in F$ containing the coalescence node r and pertaining to its section U. Thus, no subgraph whatever is reweighted in its section G.

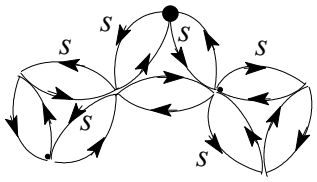
An auxiliary series $\boldsymbol{S} = \{S^j)\}_{j=0}^{\infty}$, of monodendrons now can be defined: $S^0 = K_1$, $S^1 = G = H = S$ and S^k ($k \geq 2$) is constructed in the same way as M^k above.

$S^0 = K_1$

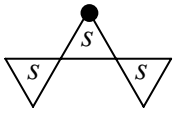


S^1

S^1



S^2

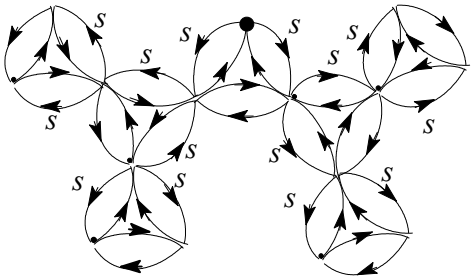


S^2

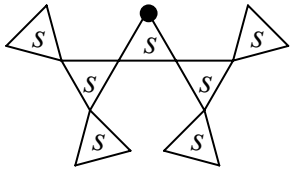
We shall use the notation J_{-r} for the graph obtained from a graph J by removing node r. Mention in passing that, in this case, $S_{-r} = U_{-r}$.

The dendrimer series $\boldsymbol{L} = \{L^j)\}_{j=0}^{\infty}$ is the series of reduced monodendrons, defined as follows: $L^0 = \mathrm{K}_0$ (an empty graph) and $L^k = S_{-r}^k$ ($k \geq 1$). It can be also introduced as a dendrimer series D

with $D^1 = G = S_{-r}$ and $H = S$.

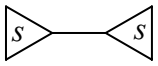


S^3

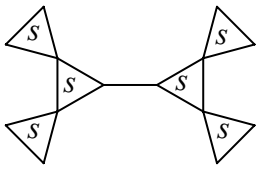


S^3

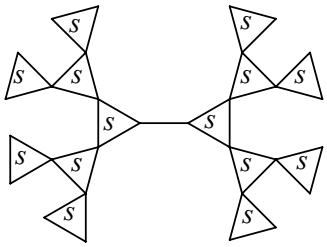
L^1



L^2

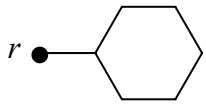


L^3

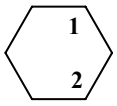


L^4

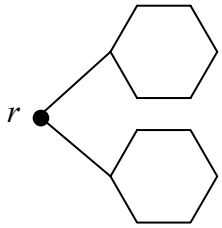
At last, we shall consider rather complicated reduced monodendrons, which will play a crucial role below. It is the series $\boldsymbol{R} = \{R^j)\}_{j=0}^{\infty}$ of dendrimers defined as follows: $R^0 = K_0$, $R_1 = G = U_{-r}$ and R^k $(k \geq 2)$ is constructed in the same way as D^k above, provided that $H = U^{|s|}$ (the s–uple coalescence of s isomorphic copies of U having the convalescence node r in common).



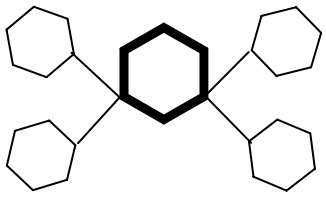
U



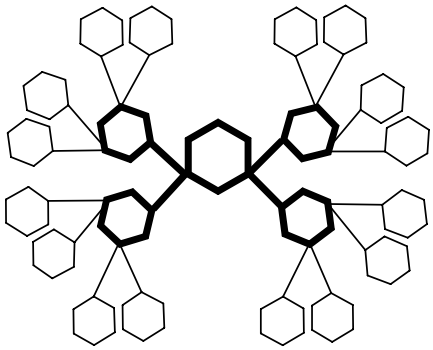
$R^1 = U_{-r}$



$H = U^{|2|}$



R^2



R^3

Choose any specific B–polynomial, whose roots comprise the corresponding B–spectrum. A

series $\boldsymbol{W} = \{W^j)\}_{j=0}^{\infty}$ of graphs is called strongly *B*–subspectral (or subspectral, for short) if the *B*–spectrum of its member W^k is wholly included in the spectrum of every member W^k ($0 \le j \le k$), taking into account the multiplicity of all eigenvalues of W^j [20]. An objective of this paper is to show that $\boldsymbol{R}$ is a universally subspectral series for all sorts of the *B*–polynomials. Now we turn to some known results that will be used below.

4 BASIC LEMMAS

We begin with a previous result (see Corollary 1.1. in [9]), rewritten here as:

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

$$B(Q;\mathbf{w}) = B(H_{-r};\mathbf{w})\,B(G;\mathbf{w}) + B(H;\mathbf{w})\,B(G_r;\mathbf{w}) - (x_r + b_r)\,B(H_{-r};\mathbf{w})\,B(G_r;\mathbf{w}) \tag{2}$$

Since the present text deals only with the homogeneous dendrimers, we have to omit here quoting the most comprehensive result of [9] (Theorem 2) and restrict our consideration to mere corollaries thereof. So, the following result is due to Corollary 2.1 in [9], viz.:

Lemma 2. Let *G* and *H* be rooted graph. Let *G*(*H*) be the graph obtained by attaching an isomorph of *H* to each of the *p* nodes of *G*. Then

$$B(G(H);x) = \left[B\left(H_{-r};x\right)\right]^p \left[B\left(G;x\right)\Big|_{x \to \frac{B\left(H^{\Delta};x\right)}{B\left(H_{-r};x\right)}} \right] \tag{3}$$

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

Note earlier specific versions of Lemma 2 for the characteristic [15,23] and matching [15] polynomials (wherein only unweighted graphs have been treated).

Recall now that any simple *B*–polynomial, such as $B(G; x)$ in (3), can be expanded in powers of *x*; therefore we can write down it as

$$B\left(G;x\right) = \gamma_0 x^p + \gamma_1 x^{p-1} + \ldots + \gamma_p x^0 \qquad (\gamma_0 = 1) \tag{4}$$

Owing to (4), we can give herein a new version of Lemma 2, viz.:

Lemma 3. Let *G* and *H* be rooted graphs. Let *G*(*H*) be rooted as above. Then

$$B\left(G\left(H\right);x\right) = \sum_{g=0}^{p} \gamma_g \left[B\left(H^{\Delta};x\right)\right]^{p-g} \left[B\left(H_{-r};x\right)\right]^g, \tag{5}$$

where H^{Δ} is the same as above.

The next quotation (Corollary 2.2 from [9]) appears herein as:

Lemma 4. Let *G* and *H* be rooted graphs. Let *G*(*H*) be the graph by attaching an isomorph of *H* to each of the *p* nodes of *G*. Also, let λ_1, λ_2, ..., λ_p be the roots of *B*(*G*; *x*). Then

$$B\left(G\left(H\right);x\right)=\prod_{i=1}^{p}\left[B\left(H^{\Delta};x\right)-\lambda_i\,B\left(H_{-r};x\right)\right] \tag{6}$$

Notice that H^{Δ} is misprinted in the original text (Corollary 2.2 of [9]) as *H*.

We can also derive a special corollary (see Corollary 2.3 in [9]) from Lemma 4, viz.:

Lemma 5. Let 0 be a *k*–uple ($k \geq 1$) root of *B*(*G*; *x*). Then $\left[B\left(H^{\Delta};x\right)\right]^{k}$ divides $B\left(G\left(H\right);x\right)$.

Here, we cannot help stating another new lemma 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 (6), is just $B(H_{\lambda_0}; x)$, 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

$$B\left(G\left(H\right);x\right)=\prod_{i=1}^{p}B\left(H_{\lambda_i};x\right) \tag{7}$$

Note that a specific case of (7), when $B(G(H);x)$ is the characteristic polynomial of a "bundled" (comblike) graph, was anticipated in a physical text [25], which is indicative of the practical need in such mathematical results among physicists.

The next fact is simply due to the definition of the graph *S*, viz.:

Lemma 7. Let *H* and *S* be two graphs, as above. Then

$$B\left(S;\mathbf{w}\right)=s\,B\left(U;\mathbf{w}\right)-\left(s-1\right)\left(x_r+b_r\right)B\left(U_{-r};\mathbf{w}\right) \tag{8}$$

We also need in a generalized analog *T* of the graph *S*. The graph *T* is derived through the same reweighting $\left(w(\alpha)\rightarrow sw(\alpha)\right)$ from the coalescence *G o U* provided that reweighted therein are only subgraphs $\alpha \in F$ containing the coalescence node *r* and pertaining to its section *U*. Thus, no subgraph whatever is reweighted in its section *G*.

Closing this paragraph is the following generalization of the last lemma.

Lemma 8. Let *G* o *U* and *T* be two graphs, as above. Then

$$B\left(T;\mathbf{w}\right)=sB\left(G\circ U;\mathbf{w}\right)-\left(s-1\right)B\left(G;\mathbf{w}\right)B\left(U_{-r};\mathbf{w}\right) \tag{9}$$

5 MAIN RESULTS

Let $m_1(\lambda)$ and $m_2(\lambda)$ be the multiplicity 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 the eigenvalue λ for the polynomials $B(G_1; x)$ and $B(G_2; x)$.

The first our statement is quite elementary and at once follows from Lemma 1.

Proposition 9. Let $m(\lambda)$ be a common multiplicity of an eigenvalue λ for polynomials $B(H; x)$ and $B(H_{-r}; x)$. Then the multiplicity of λ in the *B*–spectra of the coalescence $G \circ H$ of graphs G and H is not less than $m(\lambda)$.

Note that, *a priori* the existence of a multiple eigenvalue λ in the *B*–spectrum of H does not yet imply that λ is an eigenvalue of H_{-r}, or conversely. Nevertheless, in the case of the characteristic polynomial and usual spectra of graphs the former implication does take place [14].

One can easily turn to the case of the multiple coalescence of graphs and state the following.

Lemma 10. Let $U^{|s|}$ be the *s*–tuple coalescence of (*s* isomorphic copies of) a graph U. Then

$$B(T;\mathbf{w}) = sB(G \circ U;\mathbf{w}) - (s-1)B(G;\mathbf{w})B(U_{-r};\mathbf{w}) \tag{10}$$

Proof. Throughout this proof, we will (for brevity) write U for $B(U; x)$ and the like, in equations. Substituting $U^{|s-1|}$ for Q in (2) and assuming $U^{|s-1|}$ to be G therein we obtain

$$\begin{aligned}
U^{|s|} &= U^{|s-1|}U_{-r} + U_{-r}^{s-1}U - (x_r + b_r)U_{-r}^{s} = \\
&U_{-r}\left[U^{|s-1|} + U_{-r}^{s-2}U - (x_r + b_r)U_{-r}^{s-1}\right] = \\
&U_{-r}\left\{U_{-r}\left[U^{s-2} + U_{-r}^{s-3}U - (x_r + b_r)U_{-r}^{s-2}\right] + U_{-r}^{s-2} - (x_r + b)\right\} = \\
&U_{-r}^{2}\left\{U^{|s-2|} + 2\left[\left(U_{-r}^{s-3}U - (x_{-r} + b_r)U_{-r}^{s-2}\right)\right]\right\} = \ldots = \\
&U_{-r}^{s-1}\left\{U + (s-1)\left[U - (x_{-r} + b_r)U_{-r}\right]\right\} = \\
&U_{-r}^{s-1}\left\{s\left[U - (x_r + b_r)U_{-r}\right] + (x_r + b_r)U_{-r}\right\}.
\end{aligned}$$

However, by virtue of Lemma 7, the last expression in braces is $B(S;x)$ (or S, in a brief notation) whence the proof is immediate.

Here, we should note that a specific case of the last lemma dealing with just the characteristic polynomial has been used in quantum chemistry, where this was qualified as "the case with one atom lying on a symmetry axis or mirror plane" [18,19]. In view of numerous possible applications, studying the *B*–spectrum of various graphs with symmetry undoubtedly deserves the most serious attention [14,18–21]. In a wider context, our research is also relevant to the said. The point is that a homogeneous monodendron (leave alone more complicated dendrimers) may sometimes possess a fairly rich group of automorphisms isomorphic to a braid group or even to the wreath product of such groups. This information could surely be of use; but since it is beyond present scope, we have to revert here to the main content.

Our working tool in this paper will be the following:

Lemma 11. Let $G \circ U^{|s|}$ be the multiple coalescence of a graph G and s isomorphic copies of a graph U, as above. Then

$$B\left(G \circ U^{|s|}; x\right) = B\left(T; x\right)\left[B\left(U_{-r}; x\right)\right]^{(s-1)}. \tag{11}$$

Proof. It is due to the definition of T and the same repetitive use of Lemma 1 as in the proof of Lemma 10.

In particular, one can derive from it the following:

Corollary 11.1. Let $G(U^{|s|})$ be the rooted product of a graph G and p copies of a graph $U^{|s|}$, as above. Then

$$B\left(G\left(U^{|s|}\right); x\right) = \prod_{i=1}^{p}\left\{B\left(U^{|s|}; x\right) - \lambda_i\left[B\left(U_{-r}; x\right)\right]^s\right\} = \left[B\left(U_{-r}; x\right)\right]^{p(s-1)}\prod_{i=1}^{p}B\left(T_{\lambda_i}; x\right), \tag{12}$$

where T_{λ_i} is defined by analogy with H_{λ_i} above.

Corollary 11.1 takes into account symmetry of $U^{|s|}$ (in the coalescence point r). As it was already mentioned above, a specific case thereof dealing with the characteristic polynomial $P\left(U^{|s|}; x\right)$ of $U^{|s|}$ was earlier employed in quantum chemistry [18,19]. Corollary 11.1 shows to what (high) degree the multiplicity of eigenvalues in the B–spectra of $G(H)$ may get provided that $H = U^{|s|}$. The role of the multiple coalescence is even more impressive in the case of the series R. We shall demonstrate this through stating our main result herein, viz.:

Theorem 12. Let R^j and $L^j\left(j \geq 1\right)$ be dendrimers of the series ***R*** and ***L***, respectively. Then

$$B\left(R^j; x\right) = B\left(L^j; x\right)\prod_{k=1}^{j-1}\left[B\left(L^k; x\right)\right]^{d^{j-k}(s-1)}, \tag{13}$$

where d and s are defined as above.

Proof. By virtue of Lemma 11, one can properly prune $d^{j-1}(s-1)$ peripheral copies of a subgraph $L_{-r} = S_{-r} = U_{-r}$ and reweight r–containing subgraphs in the remaining d^{j-1} isomorphic copies of U at the periphery, which gives a new disconnected graph with the same spectrum as R^j has. Repeating the procedure for the second time one obtains $d^{j-2}(s-1)$ pruned copies of L_{-r}^2 and the corresponding reweighted remainder of R^j, *et seq*. At the end, one obtains $d\ (s-1)$ copies of L_{-r}^{j-1} and a copy of L^j. Since successively performing these $j-1$ pruning stages exactly produces all the factors on the R.H.S. of (13), we immediately arrive at the proof.

Theorem 12 gives an important corollary, viz.:

Corollary 12.1. Let R^j and R^k $(0 \leq j \leq k)$ be two members of the series ***R***. Then the B–spectrum of R^j always contained in the B–spectrum of R^k, taking into account the multiplicity of every eigenvalue of R^j.

We can also state the second version of Corollary 12.1, viz.:

Corollary 12.2. The series ***R*** is strongly *B*–subspectral.

Now we shall turn to discussing possible applications of the above results.

6 DISCUSSION

The analysis of the above mathematical results enables us to draw the following conclusions. According to basic Lemmas 2–6 and Corollary 11.1 derived herein, the B–spectrum of the rooted product $G(H)$ (hence *F*–graphs as well) can uniquely be reconstructed from like *B–spectra* of graphs *G*, *H* and H_{-r}. Regrettably a similar reconstruction for the general dendritic series *D* is (yet) unknown. Apparently, in a hybrid case, when the role of *H* is played by a (preassembled) monodendron M^j and all vertices of *G* are employed for attachments, the *B*–spectrum of the dendrimer (or else the rooted product $G(M^j)$) thus obtained is reconstructible as well. To some degree, the last already sounds promising because otherwise it would be very difficult to predict the *B*–spectra of target graphs (respectively, molecules), as is necessary for creating substances with given electronic and photonic properties.

The main idea of the paper is using the multiple coalescence of graphs as a fundamental principle for constructing dendrimers with calculable spectra. Here, it is worthy mentioning that most syntheses described in the chemical literature [1–5] do not take into account such a possibility for building hyperbranched molecules at all. For this purpose, the easiest thing is to recall Lemma 11. This lemma demonstrates that employing the multiple coalescence $U^{|s|}$ for a graph *H* gives us dendrimers (or other graphs) with the *B*–spectra, wherein the whole *B*–spectrum of a graph U_{-r} repeats, as a subspectrum, a definite number of times (see the fractal character of dendrimers). Degeneracy of described eigenvalues, first of all, tautologically means the possibility of filling some (needed) energy levels, in a molecule or bulky material, to a rather higher degree than it takes place for undegenerate eigenvalues. The said is profitable not only for electronic and photonic properties (of such substances) 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, a surface acquires the properties of a chemical group represented by a graph U_{-r} because the latter multiply contributes to the resulting *B*–spectrum of the system obtained. To the best of our knowledge, there is no other like method to saturate the spectrum of a target product (graph) with the subspectrum pertaining to U_{-r}.

The most impressive results are obtained for the monodendron series ***R***, which is the strongly *B*–subspectral series. It is predictable that molecules corresponding to different members $R^j \ (j \geq 1)$ of a series ***R*** can compose chemical mixtures whose spectral properties are linearly dependent on partial concentrations of components. This paves the way to constructing, in the future, special

sensors and measuring tools based on such a principle. Besides, the monodendrons of the series ***R*** possess the minimum possible number of distinct eigenvalues and each their eigenvalue has the maximum possible multiplicity, as compared to other sorts of dendrimers. The latter properties of monodendrons of ***R*** seem to be indicative of that they can be adopted as building units (or *per se*) in the molecular light–harvesting antennae [4–6] having the highest possible efficiency. The chief structural feature of the molecular monodendrons R^j is this: while other sorts of dendrimers used for producing intramolecular branching polyfunctional molecular fragments (such as 1,3,5–trioxibenzene etc.), the monodendrons R^j have just monoatomic branching points (polyvalent atoms C, Si, Pt, *etc*.).

The mathematical ideas discussed in this paper concern not merely spectral properties of a few classes of molecular graphs, they also suggest broad potentials for their applications to synthetic chemistry, theoretical physics, and materials engineering.

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