# A CONTRIBUTION TO THE STUDY OF REAL GRAPH POLYNOMIALS 

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#### Abstract

Let $G$ be a graph and $C$ its circuit. Let $\alpha$ stand for the matching polynomial. Let $t$ be a real number, such that $|t| \leq 1$. We demonstrate that for certain classes of compound graphs the polynomial $\beta_{t}(G, C, x)=\alpha(G, x)-2 t \alpha(G-C, x)$ is real, i.e. that all its zeros are real.


## 1. INTRODUCTION

Let $G$ be a graph containing $n$ vertices and $m$ edges. For $k>1$ let $m(G, k)$ denote the number of ways in which $k$ independent edges can be selected in $G$. In addition to this, let $m(G, 0)=1$ and $m(G, 1)=m$. Then the matching polynomial of $G$ is defined as

$$
\alpha(G)=\alpha(G, x)=\sum_{k \geq 0}(-1)^{k} m(G, k) x^{n-2 k}
$$

The theory of the matching polynomials is nowadays well elaborated [2]. In particular, it is known that $\alpha(G)$ is a real graph polynomial [4], i.e. that all its zeros are real-valued numbers.

Consider now another polynomial defined as

$$
\beta(G, C)=\beta(G, C, x)=\alpha(G, x)-2 \alpha(G-C, x)
$$

where $C$ is a circuit of the graph $G$ and $G-C$ is the subgraph obtained by deleting all the vertices of $C$ from $G$; if $C$ is a Hamiltonian circuit of $G$, then $\alpha(G-C) \equiv 1$.

The zeros of the polynomial $\beta$ play a distinguished role in Aimara's theory of cyclic conjugation [1], [12]. It has been recently conjectured [8] that the polynomial $\beta(G, C)$ is real for all cyclic graphs $G$ and all circuits $C$ contained in them. The conjecture was supported by proving its validity for various classes of graphs [7], [8], [11], [12].

In the case of unicyclic graph $\beta(G, C)$ coincides with the characteristic polynomial. Hence we have the following elementary result.

Observation 1. If $G$ is a unicyclic graph, then $\beta(G, C)$ is a real polynomial.
The above observation may serve as a motivation for a generalization of the $\beta$-polynomial concept. Define

$$
\beta_{t}(G, C, x)=\beta_{t}(G, C)=\alpha(G, x)-2 t \alpha(G-C, x)
$$

Observation 2. If $G$ is a unicyclic graph and $-1 \leq t \leq 1$, then $\beta_{t}(G, C)$ is a real polynomial.

This result follows from the fact that it is possible to construct a weighted digraph $G^{t}$ whose characteristic polynomial coincides with $\beta_{t}(G, C)$. In order to do this, an edge of $G$ belonging to the circuit $C$ is to be exchanged by a pair of oppositely directed arcs, having weights $e^{i \theta}$ and $e^{-i \theta}$. The characteristic polynomial of $G^{t}$ obeys the relation [6], [9], [12]

$$
\begin{equation*}
\phi\left(G^{t}\right)=\alpha(G)-\left[e^{i \theta}+e^{-i \theta}\right] \alpha(G-C)=\alpha(G)-2 t \alpha(G-C) \tag{1}
\end{equation*}
$$

where $t=\cos \theta$. For $\theta$ being a real number the adjacency matrix of $G^{t}$ is Hermitean and therefore all the zeros of $\phi\left(G^{t}\right)$ are real-valued.

Examples show that when the parameter $t$ is less than -1 or greater than +1 , then the $\beta_{t}$-polynomial of a unicyclic graph may have complex-valued zeros. The simplest such example is provided by the triangle, whose $\beta_{t}$-polynomial is $x^{3}-3 x-2 t$. It is easy to verify that all the three zeros of this polynomial are real if and only if $|t| \leq 1$.

The result formulated here as Observation 2 can easily be extended to graphs possessing several circuits, such that no two circuits share a common edge [6], [9]:

Observation 3. If $G$ is a graph whose no edge belongs to more than one circuit and $-1 \leq t \leq 1$, then for all circuits $C$ of $G, \beta_{t}(G, C)$ is a real polynomial.

In what follows we show that the $\beta$-polynomials of some other polycyclic graphs are also real for all values of $t,|t| \leq 1$.

## 2. THE COMPOUND GRAPHS $G_{n}$ AND $G_{n}[]$

The one-vertex graph will be denoted by $K_{1}$ and its vertex labeled by $u_{0}$.
Let $H$ be an $n$-vertex graph and let $S$ be a subset of its vertex set. Then by $H[S]$ we denote the $(n+1)$-vertex graph obtained by connecting all elements of $S$ with the vertex $u_{0}$ of $K_{1}$.

Let $G$ be a graph and $v$ and $w$ its two (not necessarily distinct) vertices. Construct the graph $G_{n}$ by taking $n$ copies $(n>1)$ of $G$ and joining the vertex $v$

Fig. 1
of the $(j+1)$-th copy to the vertex $w$ of the $j$-th copy, $j=1,2, \ldots, n-1$ and, in addition, the vertex $v$ of the first copy to the vertex $w$ of the $n$-th copy (see Fig. 1).

The compound graph $G_{n}$ has the following obvious property: The deletion from $G_{n}$ of any vertex labeled by $v$ results in the same subgraph; this subgraph will be denoted by $G_{n}-v$.

If $G$ is a tree then $G_{n}$ is unicyclic and its unique circuit will be denoted by $C^{*}$. Since all the vertices of $G_{n}$, labeled by $v$, necessarily belong to the circuit $C^{*}$, the subgraph $G_{n}-v$ is acyclic (but needs not be connected).

Denote by ${ }_{n}$ and ${ }_{n}$ the sets of vertices of $G_{n}$ labeled by $v$ and $w$, respectively (see Fig. 1). The cardinalities of these sets are, of course, equal to $n$.

Lemma 1. For any $\subseteq_{n}$,

$$
\begin{equation*}
\alpha\left(G_{n}[]\right)=x \alpha\left(G_{n}\right)-\| \alpha\left(G_{n}-v\right) \tag{2}
\end{equation*}
$$

where || stands for the cardinality of the set.

$$
\text { If }=\varnothing \text { then } G_{n}[] \text { is isomorphic to the disconnected graph } G_{n} \cup K_{1} .
$$

Because of the identity [2], [5]

$$
\begin{equation*}
\alpha\left(H_{a} \cup H_{b}\right)=\alpha\left(H_{a}\right) \alpha\left(H_{b}\right) \tag{3}
\end{equation*}
$$

and the fact that $\alpha\left(K_{1}\right)=x$, in the case when is the empty set, eq. (1) is satisfied in a trivial manner.

It remains, therefore, to examine only the case when the set is non-empty.
If $e$ is an edge of the graph $H$, connecting the vertices $p$ and $q$, then [2], [5],

$$
\begin{equation*}
\alpha(H)=\alpha(H-e)-\alpha(H-p-q) \tag{4}
\end{equation*}
$$

Applying the recurrence relation (4) to an edge of $G_{n}[]$, connecting a vertex from with $u_{0}$, we obtain

$$
\alpha\left(G_{n}[]\right)=\alpha\left(G_{n}[]\right)-\alpha\left(G_{n}-v\right)
$$

where $^{\prime}=\backslash\{v\}$. If ${ }^{\prime}$ is non-empty, then the application of (4) has to be repeated to the edge of the graph $G_{n}[']$, connecting $u_{0}$ and $v^{\prime}, v^{\prime} \in^{\prime}$. This yields

$$
\alpha\left(G_{n}[]\right)=\alpha\left(G_{n}\left[^{\prime \prime}\right]\right)-2 \alpha\left(G_{n}-v\right)
$$

where " $=\backslash\left\{v, v^{\prime}\right\}$. If " is non-empty then the procedure has to be repeated again, etc. Ultimately we arrive at

$$
\alpha\left(G_{n}[]\right)=\alpha\left(G_{n} \cup K_{1}\right)-\| \alpha\left(G_{n}-v\right)
$$

Lemma 1 follows now from eq. (3).

In a fully analogous manner we may deduce
Lemma 2. Let $G-v$ and $G-w$ be isomorphic graphs and $v \neq w$. Then for any $\subseteq{ }_{n}$ and $\subseteq{ }_{n}$

$$
\alpha\left(G_{n}[\cup]\right)=x \alpha\left(G_{n}\right)-(\|+\|) \alpha\left(G_{n}-v\right) .
$$

According to Lemmas 1 and 2 the matching polynomials of $G_{n}[]$ and $G_{n}[\cup]$ are independent of the actual choice of the vertices to which the vertex $u_{0}$ is connected and depend only on their number, i.e. on the cardinalities of the sets and.

## 3. AN AUXILIARY WEIGHTED DIGRAPH

Denote by $\phi(H)=\phi(H, x)$ the characteristic polynomial of the graph $H$. Suppose that the vertices $p$ and $q$ of $H$ are connected by an edge $e$ and that the weight of this edge is $k$. A well known result of graph spectral theory [3] is the relation

$$
\begin{equation*}
\phi(H)=\phi(H-e)-k^{2} \phi(H-p-q) \tag{5}
\end{equation*}
$$

which holds provided $e$ is a bridge. (Recall that an edge $e$ is said to be a bridge of the graph $H$ if $H-e$ has more components than $H$.) Another well known identity for the characteristic polynomial is [3]

$$
\begin{equation*}
\phi\left(H_{a} \cup H_{b}\right)=\phi\left(H_{a}\right) \phi\left(H_{b}\right) \tag{6}
\end{equation*}
$$

Let ${ }^{1}$ be a one-element subset of ${ }_{n}$. Then $G_{n}\left[{ }^{1}\right]^{k}$ denotes the graph obtained from $G_{n}\left[{ }^{1}\right]$ by associating the weight $k$ to the edge $e_{0}$ which connects the vertex $u_{0}$ with the vertex $v \in{ }^{1}$. Observe that $e_{0}$ is a bridge.

As already pointed out, if $G$ is a tree then $G_{n}$ is unicyclic and its unique circuit is denoted by $C^{*}$. If $G$ is a tree then $G_{n}^{t}\left[{ }^{1}\right]^{k}$ denotes the digraph obtained from $G_{n}\left[{ }^{1}\right]^{k}$ by exchanging an edge (any edge) belonging to $C^{*}$ by a pair of oppositely directed arcs, having weights $e^{i \theta}$ and $e^{-i \theta}, t=\cos \theta$.

Applying eq. (5) to the edge $e_{0}$ of $G_{n}^{t}[]^{k}$ and bearing in mind eq. (6) as well as $\phi\left(K_{1}\right)=x$, we immediately arrive at

Lemma 3. If $G$ is a tree then

$$
\phi\left(G_{n}^{t}\left[{ }^{1}\right]^{k}\right)=x \phi\left(G_{n}^{t}\right)-k^{2} \phi\left(G_{n}-v\right)
$$

Further, as a special case of eq. (1) we have
Lemma 4. If $G$ is a tree then

$$
\phi\left(G_{n}^{t}\right)=\alpha\left(G_{n}\right)-2 \operatorname{ta} \alpha\left(G_{n}-C^{*}\right)
$$

## 4. THE MAIN RESULTS

Theorem 1. If $G$ is a tree, then for all $t,-1 \leq t \leq 1$, all $n>1$ and all $\subseteq n$,

$$
\left.\beta_{t}\left(G_{n}[], C^{*}\right)=\phi\left(G_{n}^{t}[]^{1}\right]^{k}\right)
$$

with $k=\sqrt{\|}$.
Theorem 2. Let $G-v$ and $G-w$ be isomorphic graphs and $v \neq w$. If $G$ is a tree, then for all $t,-1 \leq t \leq 1$, all $n>1$, all $\subseteq_{n}$ and all $\subseteq_{n}$,

$$
\beta_{t}\left(G_{n}[\cup], C^{*}\right)=\phi\left(G_{n}^{t}\left[^{1}\right]^{k}\right)
$$

with $k=\sqrt{\|+\|}$.
From the definition of the $\beta_{t}$-polynomial,

$$
\beta_{t}\left(G_{n}[], C^{*}\right)=\alpha\left(G_{n}[]\right)-2 \operatorname{ta} \alpha\left(G_{n}-C^{*} \cup K_{1}\right)
$$

Using eq. (3) and the fact that $\alpha\left(K_{1}\right)=x$ we get

$$
\beta_{t}\left(G_{n}[], C^{*}\right)=\alpha\left(G_{n}[]\right)-2 x t \alpha\left(G_{n}-C^{*}\right)
$$

which combined with Lemma 1 yields

$$
\begin{equation*}
\beta_{t}\left(G_{n}[], C^{*}\right)=x\left[\alpha\left(G_{n}\right)-2 t \alpha\left(G_{n}-C^{*}\right)\right]-\| \alpha\left(G_{n}-v\right) \tag{7}
\end{equation*}
$$

If a graph $H$ is acyclic, then [2], [5], $\phi(H) \equiv \alpha(H)$. Consequently, $\alpha\left(G_{n}-v\right) \equiv$ $\phi\left(G_{n}-v\right)$. Bearing this fact in mind and using Lemma 4, the right-hand side of (7) is readily transformed into

$$
\beta_{t}\left(G_{n}[], C^{*}\right)=x \phi\left(G_{n}^{t}\right)-\| \alpha\left(G_{n}-v\right)
$$

Theorem 1 follows now from Lemma 3 .
Proof of Theorem 2 is analogous, except that instead of Lemma 1 we now have to employ Lemma 2.

All the zeros of the characteristic polynomial of the auxiliary weighted digraph $G_{n}^{t}\left[^{1}\right]^{k}$ are real-valued [3]. Therefore we have

Corollary 1.1. Under the conditions specified in Theorem 1, $\beta_{t}\left(G_{n}[]\right)$ is a real polynomial.
Corollary 2.1. Under the conditions specified in Theorem $2, \beta_{t}\left(G_{n}[\cup]\right)$ is a real polynomial.

Theorems 1 and 2 can be further extended. Let the graphs $G_{n}[] T$ and $G_{n}^{t}\left[{ }^{1}\right]^{k} T$ be obtained by identifying the vertex $u_{0}$ of $G_{n}[]$ and $\left.G_{n}^{t}{ }^{1}\right]^{k}$, respectively, with the root of a rooted tree $T$. Then we can prove the following results.

Theorem 3. Let $T$ be an arbitrary rooted tree. Theorem 1 remans valid if $G_{n}[]$ and $G_{n}^{t}\left[{ }^{[1}\right]^{k}$ are exchanged by $G_{n}[] T$ and $G_{n}^{t}\left[{ }^{1}\right]^{k} T$, respectively.

Theorem 4. Let $T$ be an arbitrary rooted tree. Theorem 2 remains valid if $G_{n}[\cup]$ and $\left.G_{n}^{t}[]^{1}\right]^{k}$ are exchanged by $G_{n}[\cup]$ and $G_{n}^{t}[]^{1} T$, respectively.

Theorems 3 and 4 imply that under conditions specified in Theorems 1 and 2, $\beta_{t}\left(G_{n}[] T, C^{*}\right)$ and $\beta_{t}\left(G_{n}[\cup] T, C^{*}\right)$ are real polynomials for all rooted trees $T$ and for all values of the parameter $t,-1 \leq t \leq 1$.

Remark. The special case of Theorems 1 and 3, when the vertices $v$ and $w$ coincide and when $t=1$ was previously reported by the author in [7].

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## REFERENCES

(1977), 2048-2053.
2. : Recent Results in the Theory of Graph Spectra. North-Holland, Amsterdam, 1988.
3. :Spectra of Graphs - Theory and Application. Academic Press, New York, 1980. Ontario, 1984, 281-293.
5. 5 (1981), 137-597.
6. : Difficulties with topological resonance energy. Chem. Phys. Letters, 66 (1979), 595-597.
7. : A real graph polynomial? Graph Theory Notes, New York, 22 (1992), 33-37.
8.
: A property of the circuit characteristic polynomial. J. Math. Chem., 5 (1990), 81-82.
9. : Cyclic conjugation and the Hückel molecular orbital model. Theor. Chem. Acta, 60 (1981), 203-226.
10.
gation and an example supporting its validity. Submitted for publication.
11.
theory of cyclic conjugation. J. Serb., Chem. Soc., 55 (1990), 193-198.
12. : Circuit resonance energy. On the roots of circuit characteristic polynomial. Bull. Chem. Soc. Japan, 63 (1990), 765-769.

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