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On the Calculation of the Acyclic Polynomial

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Graphical methods are developed for recursive evaluation of the acyclic polynomial. Analytical formulas of the acyclic polynomials for several specific series of graphs are given. Mathematical properties of the derivatives of the acyclic polynomial are given.

Key words: Acyclic polynomial – Graph theory – Topological index

1. Introduction

The non-adjacent numbers $p(G, k)$ are defined [1] as the number of ways in which k mutually non-incident edges can be selected in a graph G. Further, the Z-counting polynomial $Q_G(X)$ and the topological index Z_G are introduced as [1]

$$Q_G(X) = \sum_{k=0}^{m} p(G, k)X^k \tag{1}$$

and

$$Z_G = Q_G(1) = \sum_{k=0}^{m} p(G, k). \tag{2}$$

Although these quantities were initially supposed to be suitable only for modelling the thermodynamic properties of saturated hydrocarbons [1, 2], applications were later found in such diverse fields as chemical documentation [3], dimer statistics [4], and number theory [5]. If G is the molecular graph of a π-electron network, then

$p(G, m) =$ number of Kekulé structures

$p(G, m-1) - m \cdot p(G, m) =$ number of Dewar structures.

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These simple identities indicate the relevance of the non-adjacent numbers in the theory of conjugated compounds. Really, the non-adjacent numbers are closely related to the coefficients of the characteristic polynomial of G [6] and therefore play an important role in the Hückel molecular orbital theory [6, 7]. In particular, the topological index was shown to be related to various HMO reactivity indices, e.g., total π-electron energy [8], bond order [9] and π-electron charge density [10].

A qualitatively new application of the non-adjacent numbers was recently developed in two independent papers [11, 12]. A quantity $P^{ac}(G, X)$, the acyclic polynomial has been introduced as

$$P^{ac} \equiv P^{ac}(G) \equiv P^{ac}(G, X) = \sum_{k=0}^{m} (-1)^k p(G, k) X^{n-2k} \tag{3}$$

where n is the number of vertices of the graph G. This topological function enables a new approach to the concept of Dewar resonance energy [11, 12].

There is an evident relation between $Q_G(X)$ and $P^{ac}(G, X)$, namely,

$$P^{ac}(G, X) = X^n Q_G(-X^{-2}). \tag{4}$$

Therefore, both the polynomials Q_G and P^{ac} contain the same topological information and fulfill closely analogous recurrence relations. Nevertheless, there are two distinguished properties of the acyclic polynomials which are worth mentioning.

- If, and only if the graph is acyclic, its acyclic polynomial coincides with the characteristic polynomial[1].
- All roots of all acyclic polynomials are real[2].

A graphic recursion method was proposed for the calculation of the Z-counting polynomial [1, 6]. Because of Eq. (4), this method is equally well applicable in the case of the acyclic polynomial [11, 14, 16]. In the present work we shall develop a few new graphic techniques for evaluation of P^{ac}. Furthermore, we hope that the obtained results enable a deeper insight into, and a better understanding of the topological and algebraic properties of the acyclic polynomial. Additional mathematical properties of P^{ac} are discussed elsewhere [14].

2. Recurrence Formulas for the Acyclic Polynomial

The basic recurrence relation for the graphic evaluation of P^{ac} is

$$P^{ac}(G) = P^{ac}(G-e) - P^{ac}(G \ominus e) \tag{R1}$$

where $G-e$ is obtained by deletion of the edge e from G and $G \ominus e$ is obtained by deletion of the edge e and the both vertices incident to it. Hence, $G-e$ and $G \ominus e$

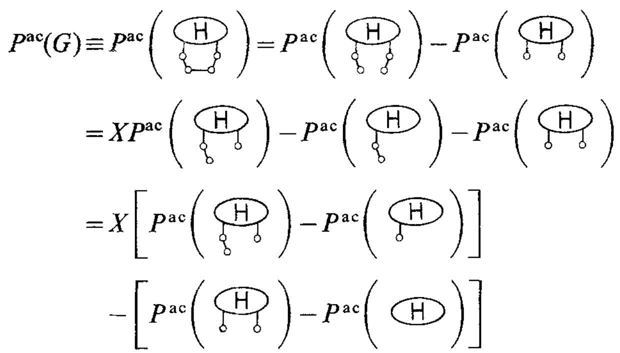
[1] For further details see [13] and [14] and references cited therein.

[2] This property of the acyclic polynomial has not yet been proved and should be a challenge for the mathematicians. Its validity is now checked by computers on several thousands of graphs [15].

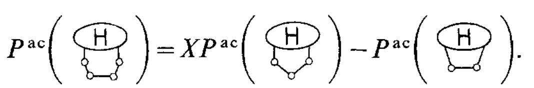
possess n and $n-2$ vertices, respectively. Various proofs of (R1) are given in Refs. [1, 14, 16].

Although (R1) provides a universal algorithm for the evaluation of P^{ac}, its application is not simple in the general case. We derive now a few specializations of (R1) which may be useful if the considered graph possesses a particular structural detail. At the same time these results exhibit interesting topological properties of P^{ac}

Let us first consider graph G containing two adjacent vertices of degree two. Then

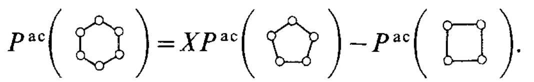


and finally,



(R2)

In the above formulae H denotes an arbitrary subgraph of G. The identity (R2) presents in fact a "ring contraction" procedure. For example,



Assume now that v is a vertex of degree d. Let v be incident to the edges $e_1, e_2, \ldots, e_d$. Then

$$\begin{aligned} P^{ac}(G) &= P^{ac}(G-e_1) - P^{ac}(G \ominus e_1) \\ &= P^{ac}(G-e_1-e_2) - P^{ac}(G \ominus e_1) - P^{ac}(G \ominus e_2) \\ &= \cdots \\ &= P^{ac}(G-e_1-e_2-\cdots-e_d) - \sum_{j=1}^{d} P^{ac}(G \ominus e_j). \end{aligned}$$

Since it is evident

$$P^{ac}(G-e_1-e_2-\cdots-e_d) = XP^{ac}(G-v),$$

it follows,

$$P^{ac}(G) = XP^{ac}(G-v) - \sum_{j=1}^{d} P^{ac}(G \ominus e_j). \qquad \text{(R3)}$$

Let us now divide the edges incident to the vertex v into two arbitrary parts $f_1, f_2, \ldots, f_a$ and $g_1, g_2, \ldots, g_b$ with $a+b=d$. Then,

$$P^{\mathrm{ac}}(G)=P^{\mathrm{ac}}(G-f_1-f_2-\cdots-f_a)-\sum_{j=1}^{a} P^{\mathrm{ac}}(G\ominus f_j) \tag{5}$$

$$P^{\mathrm{ac}}(G)=P^{\mathrm{ac}}(G-g_1-g_2-\cdots-g_b)-\sum_{j=1}^{b} P^{\mathrm{ac}}(G\ominus g_j). \tag{6}$$

The sum of Eqs. (5) and (6) is

$$2P^{\mathrm{ac}}(G)=P^{\mathrm{ac}}(G-f_1-f_2-\cdots-f_a)+P^{\mathrm{ac}}(G-g_1-g_2-\cdots-g_b) - \sum_{j=1}^{d} P^{\mathrm{ac}}(G\ominus e_j). \tag{7}$$

Subtracting (R3) from (7) one obtains

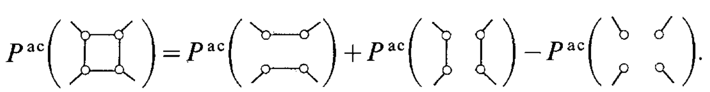
$$P^{\mathrm{ac}}(G)=P^{\mathrm{ac}}(G-f_1-\cdots-f_a)+P^{\mathrm{ac}}(G-g_1-\cdots-g_b)-XP^{\mathrm{ac}}(G-v). \tag{R4}$$

In particular, for $a=1$ we have

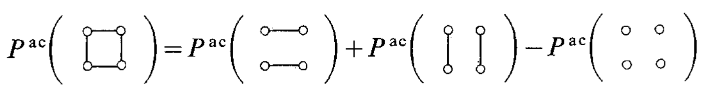
$$P^{\mathrm{ac}}(G)=P^{\mathrm{ac}}(G-e_1)-XP^{\mathrm{ac}}(G-v)+P^{\mathrm{ac}}(G-e_2-\cdots-e_d).$$

An important algebraic consequence of (R4) will be discussed in the last section.

By an analogous, but more tedious way of reasoning, the following relation can be obtained for graphs possessing a 4-membered cycle.



For example,



$$=(X^2-1)^2+(X^2-1)^2-X^4$$
$$=X^4-4X^2+2.$$

3. Analytical Formulas of the Acyclic Polynomials for Several Specific Examples

Several specific examples will be given here. The P^{ac} of a pass progression P_n corresponding to the carbon atom skeleton of the polyene with n carbon atoms is identical to its characteristic polynomial as

$$P^{\mathrm{ac}}(P_n)=\sum_{k=0}^{[n/2]}(-1)^k\binom{n-k}{k}X^{n-2k}. \tag{8}$$

The coefficients of the P^{ac} of a cycle C_n with n points has been derived in Ref. [1] as

$$P^{\mathrm{ac}}(C_n)=\sum_{k=0}^{[n/2]}(-1)^k\frac{n}{n-k}\binom{n-k}{k}X^{n-2k}. \tag{9}$$

The graph corresponding to an alternant hydrocarbon is a subgraph of a bicomplete graph or a complete bipartite graph K_{n_1,n_2} composed of n_1 starred and n_2 unstarred atoms together with all the possible combination bonds of starred and unstarred atom pairs. The P^{ac} of graph K_{n_1,n_2} can be derived as follows. Let v_1 and v_2 be atoms respectively chosen from the starred and unstarred groups in K_{n_1,n_2}. Let also e_j be an arbitrary bond connecting both the groups of atoms. Immediately one gets

$$K_{n_1,n_2}-v_1=K_{n_1-1,n_2}, \qquad K_{n_1,n_2}-v_2=K_{n_1,n_2-1}, \quad \text{and}$$
$$K_{n_1,n_2}\ominus e_j=K_{n_1-1,n_2-1}.$$

Then from (R3) the following recurrence formula is obtained,

$$\begin{aligned} P^{\mathrm{ac}}(K_{n_1,n_2}) &= XP^{\mathrm{ac}}(K_{n_1-1,n_2})-n_2P^{\mathrm{ac}}(K_{n_1-1,n_2-1}) \\ &= XP^{\mathrm{ac}}(K_{n_1,n_2-1})-n_1P^{\mathrm{ac}}(K_{n_1-1,n_2-1}). \end{aligned}$$

Successive application of these relations yields

$$\begin{aligned} P^{\mathrm{ac}}(K_{n_1,n_2}) &= (X^2-n_1-n_2+1)P^{\mathrm{ac}}(K_{n_1-1,n_2-1}) \\ &\quad -(n_1-1)(n_2-1)P^{\mathrm{ac}}(K_{n_1-2,n_2-2}). \end{aligned}$$

Further, the following expression can be proved by induction:

$$\begin{aligned} P^{\mathrm{ac}}(K_{n_1,n_2}) &= \sum_{k=0}^{\min(n_1,n_2)} (-1)^k \frac{n_1!\,n_2!}{(n_1-k)!\,(n_2-k)!\,k!} X^{n_1+n_2-2k} \\ &= \sum_{k=0}^{\min(n_1,n_2)} (-1)^k k! \binom{n_1}{k}\binom{n_2}{k} X^{n_1+n_2-2k}. \end{aligned}$$

The meaning of this relation is clear. For the complete graph K_n we have

$$K_n-v=K_{n-1} \quad \text{and} \quad K_n\ominus e_j=K_{n-2}.$$

From (R3) one gets

$$P^{\mathrm{ac}}(K_n)=XP^{\mathrm{ac}}(K_{n-1})-(n-1)P^{\mathrm{ac}}(K_{n-2}).$$

Successive application of this relation followed by the mathematical induction gives

$$\begin{aligned} P^{\mathrm{ac}}(K_n) &= \sum_{k=0}^{[n/2]} (-1)^k \frac{n!}{(n-2k)!\,k!\,2^k} X^{n-2k} \\ &= \sum_{k=0}^{[n/2]} (-1)^k \binom{n}{2k} (2k-1)!!\,X^{n-2k}, \end{aligned}$$

where $(2k-1)!!=(2k-1)(2k-3)(2k-5)\cdots 3\cdot 1$. Several acyclic polynomials obtained by using these expressions are given in the Appendix.

4. The Derivatives of the Acyclic Polynomial

It is important to note that contrary to (R1)–(R3) the relation (R4) represents P^{ac} as a combination of polynomials of degree n only. In other words, $P^{ac}(G)$ can be written as a linear combination of acyclic polynomials of certain spanning subgraphs of G[3]. A repeated application of (R4) leads finally to

$$P^{ac}(G, X) = \sum_j a_j P^{ac}(T_j, X),$$

where T_j is an acyclic spanning subgraph of G, while a_j is an integer. Since the acyclic polynomial of an acyclic graph T is equal to its characteristic polynomial $P(T, X)$ [13, 14][2], it is

$$P^{ac}(G, X) = \sum_j a_j P(T_j, X)$$

and

$$\frac{d}{dX} P^{ac}(G, X) = \sum_j a_j \frac{d}{dX} P(T_j, X). \tag{10}$$

On the other hand, for any graph G, we have [17]

$$\frac{d}{dX} P(G, X) = \sum_{v=1}^{n} P(G-v, X). \tag{11}$$

Substitution of (11) back into (10) yields

$$\frac{d}{dX} P^{ac}(G, X) = \sum_{v=1}^{n} P^{ac}(G-v, X). \tag{12}$$

Hence, the identity (11) is valid not only for the characteristic, but also for acyclic polynomials. An analogous reasoning shows that Eq. (12) can be generalized for the higher derivatives of P^{ac} as follows.

$$\frac{d^s}{dX^s} P^{ac}(G, X) = \frac{1}{s!} \sum_{(v_1, \ldots, v_s)} P^{ac}(G - v_1 - \cdots - v_s). \tag{13}$$

The summation in Eq. (13) runs over all $\binom{n}{s}$ selections of s distinct vertices in graph G.

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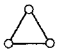
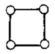
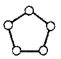
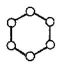
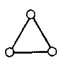
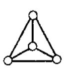
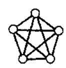
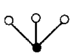
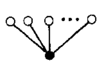
[3] A spanning subgraph of G contains all the vertices, but not all the edges of G.

Appendix

Tables of the acyclic polynomials of the fundamental graphs belonging to C_n, K_n, and K_{n_1,n_2}

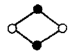
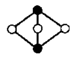
n	C_n	$P^{ac}(C_n)$	Z_G[a]
2		X^2-2	3
3		X^3-3X	4
4		X^4-4X^2+2	7
5		X^5-5X^3+5X	11
6		$X^6-6X^4+9X^2-2$	18

n	K_n	$P^{ac}(K_n)$	Z_G
1		X	1
2		X^2-1	2
3		X^3-3X	4
4		X^4-6X^2+3	10
5		X^5-10X^3+15X	26

n_1	n_2	K_{n_1,n_2}[b]	$P^{ac}(K_{n_1,n_2})$	Z_G
1	1		X^2-1	2
2	1		X^3-2X	3
3	1		X^4-3X^2	4
4	1		X^5-4X^3	5
n	1		$X^{n+1}-nX^{n-1}$	$n+1$

[a] Topological index, namely, the sum of the absolute values of the coefficients of P^{ac}.

[b] ○ and ● indicate, respectively, the starred and unstarred atoms.

n_1	n_2	K_{n_1,n_2}[b]	$P^{ac}(K_{n_1,n_2})$	Z_G
2	2		$X^4-4X2+2$	7
3	2		X^5-6X^3+6X	13
4	2		$X^6-8X^4+12X^2$	21
n	2		$X^{n+2}-2nX^n+n(n-1)X^{n-2}$	n^2+n+1
3	3		$X^6-9X^4+18X^2-6$	34
n	3		$X^{n+3}-3nX^{n+1}+3n(n-1)X^{n-1}$ $-n(n-1)(n-2)X^{n-3}$	n^3+2n+1

[b] ○ and ● indicate, respectively, the starred and unstarred atoms.

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