Acyclic and Characteristic Polynomial of Regular Conjugated Polymers and Their Derivatives$^a,b$

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A method to study the acyclic and characteristic polynomial of regular conjugated polymers is described.

For a regular polymer with $l$ bonds linking the monomer units, one first builds a $2^l \times 2^l$ polynomial matrix $T_1$. Its matrix elements are acyclic polynomials of the monomer unit graph and its subgraphs obtained by successive deletion of atoms serving as the linking sites. The acyclic polynomials of the fasciagraph (representing an open polymeric chain) and some of its subgraphs are then obtained as the appropriate matrix elements of $T_1^M$ where $M$ stands for the degree of polymerization of the polymer under consideration. For the rotagraph (representing the polymeric chain closed on itself) the acyclic polynomial equal the trace of $T_1^M$.

It is proved that the acyclic polynomials of regular polymers and some of their derivatives satisfy recursion formulae of the same form which contain $2^l + 1$ terms. The coefficients appearing in the recursion are derived only from the knowledge of the matrix $T_1$ and are, therefore, independent of $M$.

As far as the characteristic polynomial of a regular polymer is concerned, here we apply an analogon of the $T_1$-formalism only for the special case of $l = 1$ and reproduce an already known recursion formula. However, a new determinantal representation of the characteristic polynomial of a polymer as well as its explicit expression in terms of the characteristic polynomials of monomer graph and its subgraphs is established for this special case.

1. INTRODUCTION

For several decades, the pi-electronic structure of conjugated polymers has been studied by means of Hückel Molecular orbital (HMO) model. Special attention was paid to regular polymers.

It is convenient to represent conjugated polymers by graphs. They are called fasciagraphs (Latin: fascia = the band), when they represent open poly-
meric chains. In the case of the polymeric chain being closed on itself the term rotagraph (Latin: rota = the wheel) is used.¹

Two important polynomials have found applications in chemical graph theory:² the characteristic polynomial and the acyclic polynomial.

Due to the size of polymers, it is usually quite troublesome to derive their corresponding characteristic and acyclic polynomials if one starts from the basic definitions of these polynomials. In the past, the transfer matrix method (TMM)³ was used to derive the characteristic polynomial for various polymers.⁴ Another approach, mainly based on group theory, is offered in ref. 1. Recently, Kaulgud and Chitgopkar⁵ have developed a new method, the Polynomial Matrix Method (PPM), to achieve the same goal and they applied it to the calculation of the charge densities and bond orders of conjugated polymers⁶ and the total pi-electron energy of polyene chain and its derivatives.⁷ Although the PPM of Kaulgud and Chitgopkar shows some advantages as compared with TMM, it can be applied only to polymers where two monomer units are linked together by only one bond.

In the present paper, the PPM approach is generalized for any number of linking bonds 1 between the monomer units. The results are used for evaluation of the acyclic polynomial of a regular polymer and its derivatives. The corresponding recurrence formulae are also presented. As the characteristic polynomial of a regular polymer and its derivatives are concerned, the PPM approach is applied here only to polymers with \( L = 1 \).

Some properties of the graphs of polymers, i.e. the fasciagraph and the rotagraph, are described briefly in Section 2. where also some basic definitions, formulae and notations are introduced. In Section 3 and 4, the acyclic polynomial of a fasciagraph and rotagraph, respectively, is treated and the corresponding recurrence formulae are presented. The characteristic polynomial of a fasciagraph and rotagraph is discussed in Section 5. Finally, in Section 6 and 7 the acyclic and the characteristic polynomials of a fasciagraph and rotagraph, respectively, are treated and a new determinantal representation for polynomials is offered.

2. THE GRAPHS OF REGULAR POLYMERS: BASIC EQUATIONS

As already mentioned in the introduction, two graphs have been defined¹ for the description of the structure of regular polymers. The rotagraph, denoted by \( U_M \), corresponds to a polymer which is closed on itself. A schematic picture of \( U_M \) is given below: the monomeric units are depicted by small cycles; the linkage between two neighbouring monomeric units is indicated by a single line regardless of whether in a concrete polymer this linkage is achieved by one or more then one bond. \( M \) denotes the degree of polymerization, i.e., the number of monomeric units forming \( U_M \). Due to the assumed regularity of the polymer, its symmetry is at least that of the cyclic group \( C_M \); for simplicity, as is depicted below the rota-polymer may be placed on the surface of a cylinder, but such an assumption is not necessary in general. If \( M \to \infty \), the description of the polymer by \( U_M \) concides with that frequently used in solid
Using a similar formalism as there, one may factorize the characteristic polynomial of $U_M$ into exactly $M$ factors, each of them of the degree $n$ where $n$ stands for the number of vertices of the monomeric unit. The fasciagraph, $A_M$, is obtained from $U_M$ by deleting all the edges which link the monomeric unit 1 and $M$ (indicated schematically in the formalism described later.

Due to its cyclic symmetry, in the rotagraph the location of the walls of the unit cells, i.e. the fixations of the boundaries of the monomeric units, do not play any role. Thus, the rotopolymeric polyacene may be understood as being constructed from cisoid or transoid $C_4H_2$-units, as shown below but the fasciographs obtained from these two identical rotagraphs differs remarkably; the one corresponds to an ortho-quinoid, the other to a para-quinoid structure.

Obviously, the acyclic and the characteristic polynomials of these two fasciagraphs will not be identical. It is necessary to keep this in mind when applying the formalism described later.

The edges which link two neighbouring monomeric units together cross the walls of the unit cells (see above). They may be understood as the members
of a distinct cutset. Moving the walls along the direction of the propagation of the polymer, several such cutsets of different cardinality may be obtained. In the case of p-polyphenylene, there are four such cutsets which have the cardinalities 1, 2, 2, and 2 respectively:

![Diagram of cutsets](image)

According to the principles which determine the general analytical form of the characteristic polynomial, $U_M$, of the rotagraph, the linkage between two monomeric units has to be realized by cutsets of minimal cardinality, $l$. It will be convenient to impose this rule e.g. in the application of eq. (3), and we will adopt this procedure in what follows.

Let us introduce some notation and formulae required in the subsequent text.

A monomer unit containing $n$ carbon atoms is represented by the graph $A_1$ with $n$ vertices. Let vertices $s_1, s_2, \ldots, s_l$ and $r_1, r_2, \ldots, r_l$ be the linking sites for polymerization. In this way, the regular polymer, $P_M$, is obtained where $M$ stands for the degree of polymerization.

Open and closed polymeric chain are represented by a fasciagraph $A_M$ and rotagraph $U_M$, respectively. As both graphs contain $M$ monomer units each $s_i$ and $r_j$ generates a set, e.g. $\{s_i^\lambda | 1 \leq \lambda \leq M\}$. When no danger of confusion appears the index $\lambda$ is omitted.

The characteristic polynomial $\Phi(G, \lambda)$ of graph $G$ with $n$ vertices is defined as

$$\Phi(G, \lambda) = \det(\lambda I - A) = \det D$$  \hspace{1cm} (1)

where $A$ is the adjacency matrix of graph $G$ and $I$ stands for the unit matrix. The roots of $\Phi(G, \lambda)$ define the spectrum of $G$, namely the Hückel molecular orbital energies of the conjugated system represented by $G$. Using the expansion theorem of determinants, one may express $\Phi(G, \lambda)$ by

$$\Phi(G, \lambda) = \Sigma (-1)^p P (D_{11} \cdot D_{22} \cdot D_{33} \cdot \ldots \cdot D_{nn}) \hspace{1cm} (1a)$$

where $D_{ii} = (\lambda I - A)_{ii}$, $P$ is a permutation operator acting on the second indices, $p$ is the number of transpositions which produce the considered permutation $P$, and the summation runs over all the $n!$ permutations which form the symmetric group $S_n$. 
The acyclic or matching polynomial \( a(G, \lambda) \) of graph \( G \) with \( n \) vertices is defined by

\[
a(G, \lambda) = \sum_{k=0}^{[n/2]} (-1)^k p(G, k) \lambda^{n-2k}
\]

where \( p(G, k) \) is the number of \( k \)-matchings in \( G \), i.e. the number of ways in which one can select \( k \) independent edges in \( G \). In view of eq. (1), obviously in the \( p(G, k) \)'s just that contributions of the expansion theorem of determinants are collected where the permutations applied have the cycle structure \([1]\ [2]^m, n-2m, m = 1, 2, \ldots\)

The roots of \( a(G, \lambda) \) define the acyclic spectrum of \( G \) which has found some use in the study of the resonance energy of the conjugated systems\(^9\). The usefulness of such an approach is still under dispute\(^10\), however, the acyclic polynomial by itself is useful in the study of some combinatorial problems as the enumeration of valence structures for conjugated radical cations\(^11\) and others.

Recently, both polynomials have unified to the more general \( \mu(G, \lambda; t) \) polynomial\(^12\) which reduces to the earlier ones

\[
a(G, \lambda) = \mu(G, \lambda; t = 0)
\]

\[
\Phi(G, \lambda) = \mu(G, \lambda; t = 1)
\]

by an appropriate choice of the parameter \( t \).
For the sake of brevity, the following abbreviations will be used in the subsequent text: \( G^p \) denotes the subgraph obtained by deletion of the vertex \( p \) (and incident edges) from \( G \), \( G^{p(q)} \) is the subgraph obtained by deletion of the edge \((pq)\) from \( G \), \( G^{pq} \) is the subgraph obtained by deletion of the vertices \( p \) and \( q \) and their incident edges, and \( G^Z \) stands for the subgraph obtained by deletion of all vertices of the cycle \( Z \) from \( G \).

Further, since no confusion can arise, the polynomials \( \Phi(G, \lambda) \) and \( \alpha(G, \lambda) \) will be abbreviated by \( \overline{G} \) and \( G \), respectively.

The material presented has been obtained by the systematic use of a recursion formula for characteristic polynomials originally derived by Heilbronner.\(^8\) Applied to an edge \((pq)\) of the graph \( G \), it reads as

\[
\overline{G} = \overline{G^{pq}} - \overline{G^{pq}} - 2 \sum_{a} \overline{G^a} \alpha
\]  

(3)

where the summation goes over all cycles \( Z_a \) containing the edge \((pq)\).

The analogous recursion formula for evaluation of the acyclic polynomial is given by\(^9\)

\[
G = G^{pq} - G^{pq}
\]  

(4)

In the case the edge \((pq)\) is a bridge, the third term on the right side of eq. (3) equals zero and the characteristic polynomial can be treated formally in the same way as the acyclic polynomial. This idea will be used in the evaluation of the characteristic polynomial of regular polymers with a single edge connecting monomer units (Sections 6 and 7).

3. THE ACYCLIC POLYNOMIAL OF A FACSIAGRAPH

Our method to study the acyclic polynomial of a fasciagraph is based on a systematic application of the recursion formula (4) to the edges connecting monomer units.

First, it will be applied to the edges connecting the \((M - 1)\) th and \( M \) th monomer unit in \( A_M \). After it has been applied \( l \) times, once for each edge, altogether \( N = 2^l \) terms are obtained. In each of them, all \( l \) edges are deleted, and, hence, all the terms have one factor referring to \( A_{M-1} \) and its subgraphs and another one arising from the \( M \)-th unit which is expressed by \( A_1 \) and the appropriate subgraphs of \( A_1 \). By deletion of edges together with their incident vertices the two factors are simply related. For each right vertex \( r_j \) deleted from \( A_{M-1} \) the left vertex \( s_j \) has to be deleted from \( A_1 \). In \( \begin{pmatrix} 1 \\ 0 \end{pmatrix} \) of the terms no edge together with its incident vertices is deleted, in \( \begin{pmatrix} 1 \\ 1 \end{pmatrix} \) of them one edge together with its incident vertices is deleted, generally, in \( \begin{pmatrix} 1 \\ k \end{pmatrix} \) terms \( k \) edges together with their incident vertices are deleted.

As the result, one has

\[
A_M = A_1 A_{M-1} - \sum_{1 \leq h \leq l} A_1 j_1 A_{M-1} j_1 + \sum_{1 \leq h < k \leq l} A_1 j_1 j_2 A_{M-1} j_1 j_2 + \cdots + (-1)^k \sum_{1 \leq h < k < \cdots < k \leq l} A_1 j_1 j_2 \cdots j_k A_{M-1} j_1 j_2 \cdots j_k + \cdots + (-1)^l A_1 s_1 s_2 \cdots s_l
\]  

\[
A_{M-1} r_1 r_2 \cdots r_l
\]  

(5)
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$A_M$ is expressed as a combination of $N$ acyclic polynomials $A_{M-1}$, $A_{M-1}^p$, ..., $A_{M-1}^{p_1 p_2 \ldots p_k}$ with the coefficients being the acyclic polynomials of the monomer unit graph and some of its subgraphs, $A_{1}$, $A_{1}^p$, ..., $A_{1}^{p_1 p_2 \ldots p_k}$, respectively.

The recursion formula (4) could be applied to any one of the $N$ acyclic polynomials $A_{M-1}$, $A_{M-1}^p$, ..., $A_{M-1}^{p_1 p_2 \ldots p_k}$, as well, where the $r_j$'s are deleted from the $M$-th unit. Generally, one has

$$A_M = A_M^1 + \sum_{1 \leq j_1 < j_2 < \ldots < j_k \leq l} A_1^1 j_1 \ldots j_k A_{M-1}^1 j_1 \ldots j_k A_{M-1}^{p_1 p_2 \ldots p_k}$$

and, as before, any of $A_M^1 j_1 \ldots j_k$ is expressed as a combination of the same $N$ acyclic polynomials $A_{M-1}^1$, $A_{M-1}^{p_1}$, ..., $A_{M-1}^{p_1 p_2 \ldots p_k}$ but with the appropriate change of the coefficients which represent acyclic polynomials of the monomer unit graph and some of its subgraphs. The following expressions many be written for $A_M^{s_1}$, ..., $A_M^{s_1 s_2}$, ..., where the $s_j$'s are deleted from the first unit.

In total there are $N-1$ subgraphs derived from $A_M$ by deleting some of the $s_j$'s from the first and/or some of the $r_j$'s from the last unit. In that what follows the term »fasciagraph and its subgraphs« refer to this set.

In order to write the expressions in a compact way, let us introduce the index set $I = \{1, 2, \ldots, l\}$ parallel to the sets of vertices $R = \{r_1, r_2, \ldots, r_l\}$ and $S = \{s_1, s_2, \ldots, s_l\}$. Obviously, there is an one-to-one mapping of $I$ onto $R$ and onto $S$ respectively: $i \leftrightarrow r_i$, $i \leftrightarrow s_i$. Let $P(I)$ denote the partitive set of $I$, namely, the collection of all the subsets of $I$ including $I$ itself and the empty set $\emptyset$ as well:

$$P(I) = \{\emptyset, \{1\}, \{1, 2\}, \ldots, \{1, 2, 3\}, \ldots, I\} = \{I_k | 1 \leq k \leq N\}$$

Elements of $P(I)$ are denoted by $I_k$, $k = 1, 2, \ldots, 2^l$, where $I_1 = \emptyset$. The partitive sets $P(R)$ and $P(S)$ could be formed in a completely analogous manner

$$P(R) = \{r_j | J \subset I\} = \{o_k | 1 \leq k \leq N\}, \quad r_j = \{r_j | j \in J\}$$

$$P(S) = \{s_j | J \subset I\} = \{o_k | 1 \leq k \leq N\}, \quad s_j = \{s_j | j \in J\}$$

Again, obviously there is an one to one mapping of $P(I)$ onto $P(R)$ and onto $P(S)$, respectively, the elements of $P(R)$ and $P(S)$ are assumed to be ordered such that $I_k \leftrightarrow o_k$, $I_1 \leftrightarrow o_1$. Then $o_1 = \sigma_1 = \emptyset$, etc.; the cardinalities of the subsets $I_k$, $o_k$, and $o_1$ equal each other $|I_k| = |o_k| = |o_1|$. When all the vertices of $o_1$ and $o_1$ are deleted from graph $G$, a subgraph $G^o$ is obtained. Its acyclic polynomials are denoted by the same symbol as there is no danger of confusion. Since $o_1$ and $o_1$ denote empty sets, we have $G^o o_1 = G$, $G^o o_1 = G^o$ and $G^o o_1 = G^o$.

The notation introduced above enables us to rewrite eqs. (6) as follows:

$$[A_{M-1}^p, A_M^p, \ldots, A_M^{s_1 s_2 \ldots s_l}] = T_1 [A_{M-1}^p, A_{p_2}, \ldots, A_{s_1 s_2 \ldots s_l} - 1]$$

(8)
where \([ \ ]^t\) denotes a one-column matrix and the \(N \times N\) polynomial matrix \(T_1\) is defined by

\[
(T_1)_{ij} = (-1)^{|c_j|} A_1^{p_i} c_i
\]  

(9)

Applying eq. (8) to the vector \([A_{M-2}^p, \ldots, A_1^p, A_0^p, A_{M-1}^p, \ldots, A_0^p, N]^t\) one obtains

\[
[A_{M}^p, \ldots, A_1^p, A_0^p, \ldots, A_0^p, N]^t = T_1^M [A_{M-2}^p, \ldots, A_1^p, A_0^p, \ldots, A_0^p, N]^t
\]

(10)

Therefore, eq. (8) applied \(M\) times gives

\[
[A_{M}^{p_1}, A_{M}^{p_2}, \ldots, A_1^p N]^t = T_1^M [A_{0}^{p_1}, A_{0}^{p_2}, \ldots, A_0^p N]^t
\]

where the elements \(A_0^p, \ldots, A_0^p\), are, obviously, the numbers.

Inspection of eqs. (8) for \(M = 1\) gives the following initial conditions,

\[
A_1 = A_0^{p_1} = 1, \quad A_0 = A_0^{p_2} = \ldots = A_0^p N = 0
\]

(11)

and eq. (10) becomes

\[
[A_{M}^{p_1}, A_{M}^{p_2}, \ldots, A_1^p N]^t = T_1^M [1, 0, \ldots, 0]
\]

(12)

The procedure used from eq. (5) to eq. (12) could be applied to any of the \(A_1^p i^\sigma j, j = 1, 2, \ldots, N\), as well, thus giving

\[
A_1^p i^\sigma j = \sum_{k=1}^{N} (-1)^{|\sigma| k} A_1^p i^\sigma k A_{M-1}^p k^\sigma j; \quad i = 1, 2, \ldots, N
\]

(13)

Note that the set \(\sigma_j\) is deleted from the first and the set \(\sigma_i\) from the last monomer unit. Inspection of eqs. (13) for \(M = 1\) determines the initial conditions as follows:

\[
(-1)^{|\sigma_j|} A_0^0 \sigma_j = \delta_{ij},
\]

hence,

\[
T_0 = I.
\]

(14)

Finally, one writes the relationship between the acyclic polynomials of a fasciagraph and its subgraphs and the acyclic polynomials of a monomer unit graph and its subgraphs in the following matrix form:

\[
T_M = T_1^M,
\]

(16)

where the \(N \times N\) polynomial matrix \(T_M\) is given by

\[
(T_M)_{ij} = (-1)^{|\sigma_j|} A_1^0 \sigma_j
\]

(17)

Eq. (16) can be regarded as a generalization of the Polynomial Matrix Method of Kaulgud and Chitgopkar.5,6

Let us pose the question if it is possible to relate a given polynomial \(A_1^0 \sigma_j\) to the polynomials \(A_1^0 \sigma_j, L = M - 1, M - 2, \ldots, 0\), of the lower order \(L\) but of the same type, namely, to find a recurrence relation for the acyclic polynomial of a fasciagraph and its subgraphs. The solution to this is offered as follows:

Let us consider the \(N \times N\) polynomial matrix \(T_1\) and its \(N\) th order characteristic polynomial \(\Phi(T_1, \lambda)\).
The following abbreviation for the minor of the $k$th order of $T_1$ is also introduced:

$$T_1 \left( \begin{array}{ccc} i_1 & i_2 & \cdots & i_k \\ j_1 & j_2 & \cdots & j_k \end{array} \right) = \begin{vmatrix} T_{i_1 j_1} & T_{i_1 j_2} & \cdots & T_{i_1 j_k} \\ T_{i_2 j_1} & T_{i_2 j_2} & \cdots & T_{i_2 j_k} \\ \vdots & \vdots & \ddots & \vdots \\ T_{i_k j_1} & T_{i_k j_2} & \cdots & T_{i_k j_k} \end{vmatrix} \quad (18)$$

The sum of the principal minors of the order $k$ of the matrix $T_1$ is denoted by $s_k$.

$$s_k = \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq N} T_{j_1 j_2 \cdots j_k} \quad (19)$$

e.g.:

$$s_1 = \text{tr} T_1, \ s_2 = \sum_{1 < j_1 < i_2 < \cdots < i_k \leq N} T_{i_1 j_1} T_{i_2 j_2} \cdots T_{i_k j_k}, \text{ etc.} \quad (20)$$

where $\text{tr} A$ denotes the trace of the matrix $A$.

By definition there is

$$s_0 = 1 \quad (21)$$

As it is known from linear algebra, one can write $\Phi(T_1, \lambda) as^{13a}$

$$\Phi(T_1, \lambda) = \det(\lambda I - T_1) = \sum_{k=0}^{N} (-1)^k s_k \lambda^{N-k} \quad (22)$$

Applying the Cayley-Hamilton theorem,$^{13b}$

$$\Phi(T_1, T_1) = 0 \quad (23)$$

one obtains

$$\sum_{k=0}^{N} (-1)^k s_k T_1^{N-k} = 0, \quad (24)$$

which identity, after use of the basic eq. (16), has the following form:

$$\sum_{k=0}^{N} (-1)^k s_k T_{N-k} = 0 \quad (25)$$

By considering the matrix element in the $i$th row and the $j$th column of the above matrix identity, one has

$$\sum_{k=0}^{N} (-1)^k s_k A_{N-k}^{i \sigma_j} = 0, \ i = 1, 2, \ldots, N, j = 1, 2, \ldots, N \quad (26)$$

where eq. (17) has been used.

Eq. (26) represents the basic recursion formula of our paper. The question raised earlier is answered by this equation: the acyclic polynomial $A_{N, \sigma_1}^{\sigma_2}$ of the $N$th order is given by recursion containing acyclic polynomials $A_{L, \sigma_1}^{\sigma_2}$ of the same type but of lower order $L$, $L = N - 1, N - 2, \ldots, 2, 1, 0$. Moreover, the coefficients $s_k$ are the same for each choice of $\sigma_1$ and $\sigma_2$ and therefore-
all the polynomials $A_N^{0,s_i}, i = 1, 2, \ldots, N$, $j = 1, 2, \ldots, N$, obey the recursion formula of the same form. The result can be understood as the topological consequence of the fact that all the polymers $A_N^{0,s_i}$ share the common inner fragment, namely the polymer $P_{N-2}$ and its linking edges.

Multiplying eq. (24) by $T_{1}^{M-N}, M \geq N$, and taking the matrix element in the $i$ th row and $j$ th column, one obtains

$$
\Sigma_{k=0}^{N} (-1)^{k} s_{k} A_{M-k}^{0,s_{i}} = 0, M \geq N
$$

(27)

In such a way $A_{M}^{0,s_{i}}, M \geq N$ is expressed by $A_{M}^{0,s_{i}}, \ldots, A_{M}^{0,s_{i}}$ in the same form as is $A_{N}^{0,s_{i}}$ in terms of $A_{N-1}^{0,s_{i}}, \ldots, A_{0}^{0,s_{i}}$. Let us emphasise that the coefficients of the recursion formula, $(-1)^{k} s_{k}$, are independent of $M$.

Moreover, by repeated use of eq. (26) one is able to express any of the polynomials $A_{M}^{0,s_{i}}, M \geq N$ in terms of a new recursion containing only $A_{N-1}^{0,s_{i}}, A_{N-2}^{0,s_{i}}, \ldots, A_{0}^{0,s_{i}}$. This point of view, however, is of no interest in our further considerations.

The basic eq. (16) can also be written as

$$
T_{M} = T_{1} \cdot T_{M-1} = T_{M-1} \cdot T_{1}
$$

(28)

The first term on the right side describes the application of the Heilbronner-like formula (4) to the edges linking $(M-1)$ th and $M$ th monomer unit graphs in the fasciagraph $A_{M}$ as described previously while in the second term the edges linking the first and the second monomer unit graph are considered. By writing the matrix elements of identities (28), one has

$$
\Sigma_{k=0}^{N} (-1)^{k} s_{k} A_{M-k}^{0,s_{i}} = \Sigma_{k=0}^{N} (-1)^{k} s_{k} A_{M-k}^{0,s_{i}}
$$

(29)

In such a way, some relationship is established among $A_{M}^{0,s_{i}}$ and $A_{M}^{0,s_{i}}$ polynomials, $k = 1, 2, \ldots, N$, and the idea will be elaborated in more detail in Section 6 which treats fasciagrams with $l = 1$.

We would like to comment on the use of the recursive relations (26) and (27). We have adopted the following scheme: Polynomials $A_{M}^{0,s_{i}}$ are defined for $M > 0$ by their graphs while polynomials $A_{0}^{0,s_{i}}$ are given by eq. (15). Polynomials $A_{1}^{0,s_{i}}, A_{2}^{0,s_{i}}, \ldots, A_{N-1}^{0,s_{i}}$ can be easily evaluated explicitly by application of eq. (16). After that, higher order polynomials $A_{M}^{0,s_{i}}, M \geq N$, may be determined by eq. (16) or by the recurrence relations (26) and (27).

Some derivatives of polymer $A_{M}$ can be treated in the same manner.

First, let us consider the acyclic polynomials of the derivative $B_{M}$ of polymer $A_{M}$ where two terminal groups represented by graphs $U$ and $V$ are attached as is depicted below.

The terminal group $U$ is linked with the first monomer unit by $1''$ edges and the terminal group $V$ with the $M$ th monomer group by $1'$ edges. Linking sites in the first and the $M$ th monomer unit are subsets of $S$ and $R$, respectively.

Prior to further discussion, some useful definitions will be introduced.

Vertices $x_{1}, x_{2}, \ldots, x_{i''}$ form the set $X \subseteq U$. Its partitive set is $P(X)$ and the elements of $P(X)$ are denoted by $\chi_{k}, k = 1, 2, \ldots, N''$. As before $N''$ stands for $2i''$. 

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VERTICES $s(x_1), s(x_2), \ldots, s(x_{l''})$ are linked with vertices $x_1, x_2, \ldots, x_{l''}$ and form the set $S_x \subset S$. Let us construct the partitive set $P(S_x)$ in the same way as $P(X)$. Therefore, one has $|\sigma_k^{(X)}| = |\chi_k|$, where $\sigma_k^{(X)} \in P(S_x)$, $k = 1, 2, \ldots, N''$.

Similarly, starting with $Y = \{y_1, y_2, \ldots, y_i\}$ one forms its partitive set $P(Y)$ with elements denoted by $l_k$, $k = 1, 2, \ldots, N$, where $N' = 2^l$. Let us form the partitive set $P(R_Y)$ in the same way as $P(Y)$. Obviously, one has $|\sigma_k^{(Y)}| = |l_k|$ where $\sigma_k^{(Y)} \in P(R_Y)$, $k = 1, 2, \ldots, N'$.

The subgraphs obtained by deletion of the vertices $\chi_k$ and $l_k$ from terminal groups $U$ and $V$ are denoted by $U^{k''}$ and $V^{l_k}$, respectively. The corresponding acyclic polynomials are denoted by $U^{k''}$ and $V^{l_k}$ as well, as there is no danger of confusion.

By applying the recursion formula (4) successively to all the bonds connecting $U$ and $V$ with polymer $A_M$, one obtains the following expression for the acyclic polynomial of the derivative $B_M$:

$$B_M = \sum_{k'=1}^{N'} \sum_{k''=1}^{N''} (-1)^{k''} V^{l_k} (-1)^{\sigma^{(X)}} A_M^{q_k^{(X)}} U^{k''}$$

By taking the double sum inside and then applying the recursion (27) to each of the polynomials

$$A_M^{q_{k'}^{(Y)}} \sigma^{(X)}, M \geq N$$

one obtains

$$\sum_{k=0}^{N} (-1)^k s_k B_{M-k} = 0, M \geq N,$$

namely, the acyclic polynomials $B_M$, $M \geq N$, obey the same recursive relation as do the polynomials $A_M^{q_{k'}}$. As before, the coefficients in the recurrence are independent of $M$. The above result is a topological consequence of the fact that the polymers $B_M$ and $A_M^{q_{k'}}$, $M \geq N$, share the same inner fragment.

One can write eq. (30) in a more compact way. The quantities $U^{k''}, k = 1, 2, \ldots, N''$ are elements of a $N''$-dimensional (polynomial) vector. Because of
one-to-one correspondence of the elements $X_k$ and $o_k(\infty)$ of the partitive sets $P(X)$ and $P(S_X)$, one defines

$$U_k(\sigma) = \begin{cases} U_{S_k}, & o_k \in P(S_X) \\ 0, & o_k \notin P(S_X) \end{cases}$$

(32a)

and in such a way, a new $N$-dimensional vector $U$ is formed of which the $k$ th element reads

$$(U)_k = U_k(\sigma)$$

(32b)

Similarly, instead of elements $V_1^k, k = 1, 2, \ldots, N'$ of a $N'$-dimensional vector and because of one-to-one correspondence of the elements $I_k$ and $o_k(Y)$ of $P(Y)$ and $P_Y$, respectively, one defines

$$V_k(\sigma) = \begin{cases} V_{1}^k, & o_k \in P(P_Y) \\ 0, & o_k \notin P(P_Y) \end{cases}$$

(33a)

In such a way, a new $N$-dimensional vector $W$ is formed

$$(W)_k = (-1)^{o_k} V_k(\sigma)$$

(33)

Eq. (30) is now rewritten as follows:

$$B_M = \sum_{k'=1}^{N} \sum_{k''=1}^{N} (W') k' \cdot (-1)^{\sigma} k'' A_M(\sigma) k' \cdot (-1)^{\sigma} k'' (U)_{k''}$$

(34)

where $W'$ denotes the transpose of $W$. By use of eqs. (16) and (17), one finally has

$$B_M = W' T_M U = W' T_1^{M} U$$

(35)

Eq. (35) enables us to evaluate $B_M$ up to any order. However, only the first $N$ polynomials $B_0, B_1, \ldots, B_{N-1}$ have to be evaluated explicitly by use of the above equation while all the higher polynomials $B_M, M > N$, can be obtained by application of the recurrence (31). Also, note that formally

$$B_0 = W' U$$

(36)

A more general case appears when terminal groups $U$ and $V$ are linked to vertices of the first and the $M$ th monomer unit, respectively, which are not necessarily elements of sets $S$ and $R$, respectively. The corresponding fasciagraph is denoted by $C_M$ and depicted below.

Note that the recursive formula applies only to polynomials of the type $A_M(\sigma)$ so there is nothing to be gained when applying the Heilbronner-like formula to the edges linking the first and the $M$-th monomer unit with $U$ and $V$, respectively. It is more advisable to treat the union of the first repeating unit and $U$ as the terminal group $U'$, and the union of the last repeating unit and $V$ as the terminal group $V'$. One immediately writes
where
\[(U')_k = U'p_k, \quad (W')_k = (-1)^k V'q_k,\]
\[(38)\]

where \(q_k\) and \(r_k\) denote the elements of \(P(R)\) and \(P(S)\), eq. (7b), referring to the vertices deleted from \(U'\) and \(V'\), respectively, and analogously to eq. (31) the recurrence formula for acyclic polynomials of \(C_M\) takes then the following form:
\[\sum_{k=0}^{N} (-1)^k s_k C_{M-k} = 0, \quad M \geq N + 2,\]
\[(39)\]

where the initial condition is given by
\[C_2 = W'^{-1} \cdot U'.\]
\[(40)\]

The same form of recurrence formulae (27), (31) and (39) is a topological consequence of all the polymers \(A'_{M+1}, B_M\) and \(C_{M+2}, M > N\), sharing one and the same inner fragment.

4. THE ACYCLIC POLYNOMIAL OF A ROTAGRAPH

The acyclic polynomial of a rotagraph \(U_M\) is denoted by \(U_M\). When one applies the recursion (4) to the edges linking the first and the \(M\)-th monomer unit in \(U_M\), one obtains
\[U_M = \sum_{k=1}^{N} (-1)^k |A_{M+k}| A_{M+k}\]
\[(41)\]

Because of eqs. (16)—(17), one recognizes the diagonal terms of \(T_1^M\) and, therefore, one has
\[U_M = \text{tr} T_M = \text{tr} T_1^M.\]
\[(42)\]

As before, the matrices \(T_1^M\) serve to generate acyclic polynomials of \(U_M\) and, because of eq. (24), the following recurrence formula is valid for the \(U_M\)'s
The initial condition reads formally as

\[ U_0 = \text{tr } I = N \]

and the first \( N \) \( U_M \)-polynomials are produced by application of eq. (42).

Let us now insert an arbitrary fragment \( V \) in a otherwise regular rotational graph. In such a way, the following derivative, denoted by \( V_M \), is obtained

\[
\begin{align*}
V_M &= \sum_{i=1}^{N} \sum_{j=1}^{N} (-1)^{\sigma_i} \sigma_j \cdot A_{M-2}^{\sigma_i \sigma_j} (-1)^{\sigma_1} \cdot V^{\sigma_1} \\
V_2 &= \text{tr } W'
\end{align*}
\]

Let us introduce the matrix \( W' \) in the following way:

\[
(W')_{ij} = (-1)^{\sigma_i} \cdot V^{\sigma_1 \sigma_j}
\]

With the use of eqs. (16)—(17) the acyclic polynomial of \( V_M \) can be written as

\[
V_M = \text{tr} \left( T_1^{M-2} W' \right)
\]

and one gets the following recursion for polynomials \( V_M \):

\[
\sum_{k=0}^{N} (-1)^k s_k V_{M-k} = 0, \quad M \geq N + 2
\]

with the initial condition given by

\[
V_2 = \text{tr } W'
\]

Because all the systems considered, \( A_{M0}^{\sigma_1}, B_M, C_{M+2}, U_M, V_{M+2} \), share the same inner fragment, their corresponding acyclic polynomials obey the recursion formula of the same form.
5. THE CHARACTERISTIC POLYNOMIAL OF A FASCIAGRAPH AND A ROTAGRAPHER

Heilbronner’s recurrence formula for the characteristic polynomial $\bar{G}$ of a graph $G$ as applied to an edge of $G$ is given by eq. (3). Its repeated application to the edges of a fasciagraph $A_M$ soon leads to involved expressions. The source of difficulties lies in the deletion of all cycles containing the edge under consideration. However, the formulae for the characteristic polynomial of a dimer as well as of regular conjugated polymers can be derived but their structure is rather complicated and the results will be not presented here. However, for a fasciagraph $A_M$ with $l = 1$, no difficulties with the deletion of cycles are met and one is able to derive recurrence relations for $\bar{A}_M$. The subject will be treated in the next section.

When the characteristic polynomial $\bar{U}_M$ of a rotagraph $U_M$ is considered, one, again, is not encouraged to apply eq. (3).

However, for the sake of further considerations, let us make use of the cyclic symmetry of the problem. Then, polynomial $\bar{U}_M$ factorizes as follows:

$$\bar{U}_M = \prod_{j=1}^{M} \bar{A}(\omega_j)$$  (50)

where $\bar{A}(\omega_j)$ is the characteristic polynomial of the representative graph $A(\omega_j)$ and $\omega_j = \exp(i j 2 \pi / M)$, $j = 1, 2, \ldots, M, i = \sqrt{-1}$, is related to the $j$ th
irreducible representation of the cyclic group. For a given graph $A_1$ representing the repeating unit of $U_M$, the related representative graph $A(\omega_j)$ is obtained by the depicted procedure.

All the edges already presented in $A_1$ are retained in $A(\omega_j)$. In addition, the oriented edges $(r_k s_k)$, $k = 1, 2, \ldots, l$, between the linking vertices of sets $S$ and $R$ are introduced in $A(\omega_j)$ and have the following weights:

$$[A(\omega_j)]_{r_k s_k} = A_{r_k s_k} + \omega_j = \begin{cases} \omega_j, & \text{if } r_k \text{ and } s_k \text{ are not connected in } A \\ 1 + \omega_j, & \text{if } r_k \text{ and } s_k \text{ are connected in } A \end{cases} \quad (51)$$

and the oriented edges $(s_k r_k)$, $k = 1, 2, \ldots, l$, have the weights

$$[A(\omega_j)]_{s_k r_k} = [A(\omega_j)]^*_{r_k s_k} = A_{r_k s_k} + \omega_j^* \quad (52)$$

where $\omega_j^*$ denotes the complex conjugate of $\omega_j$.

6. THE ACYCLIC AND THE CHARACTERISTIC POLYNOMIAL A FASCIAGRAPH WITH $l = 1$

In fasciagrams, $A_M$, with $l = 1$ the edges linking the monomeric units are bridges. Therefore, they do not belong to any cycle of $A_M$ and, hence, applying eq. (3) to these edges the third term on the right hand side of eq. (3) vanishes. Applying eq. (3) to a linking edge of a rotagraph with $l = 1$ the cyclic term contains only cycles to which all the linking edges belong; hence, this term appears only at the first removal of a linking edge.

All the previously derived formulae reduce to especially simple form when the fasciagram $A_M$ and rotagraph $U_M$ with $l = 1$ are considered. Set $R$ contains one element $r_1 = r$ and $P(R)$ therefore contains two elements $q_1 = \emptyset, q_2 = \{r\}$; set $S$ contains one element $s_1 = s$ and $P(S)$ contains therefore two elements $\sigma_1 = \emptyset, \sigma_2 = \{s\}$. The fasciagrams studied are depicted below, where the abbreviation: $R_M = A_M^r, S_M = A_M^s, D_M = A_M^{rs}$ is introduced. For $M = 1$, we introduce the notation: $a \equiv A_1, q \equiv R_1, \sigma \equiv S_1, \delta \equiv D_1$, and the related graphs are depicted below.

Matrices $T_M$ and $T_1$, built up from the acyclic polynomials of the systems studied according to eq. (17) have the form

$$T_M = \begin{bmatrix} A_M - A_M^s \\ A_M^r - A_M^{rs} \end{bmatrix} = \begin{bmatrix} A_M - S_M \\ R_M - D_M \end{bmatrix} \quad (53)$$

$$T_1 = \begin{bmatrix} A_1 - A_1^s \\ A_1^r - A_1^{rs} \end{bmatrix} = \begin{bmatrix} a - \sigma \\ q - \delta \end{bmatrix} \quad (54)$$

and the basic eq. (16) reads as

$$\begin{bmatrix} A_M - S_M \\ R_M - D_M \end{bmatrix}^M = \begin{bmatrix} a - \sigma \\ q - \delta \end{bmatrix}$$

thus enabling us to build up acyclic polynomials of the fasciagrams studied by knowing the acyclic polynomials $a$, $q$, $\sigma$ and $\delta$ of the monomer unit $A_1$ and its subgraphs $A_1^r, A_1^s, A_1^{rs}$.

In order to apply the basic recurrence formula (27) of the paper, one has to evaluate the sums of the principal minors of the order $k$ of the matrix $T_1$. The quantities have earlier been denoted by $s_k$ and they are evaluated as follows ($k = 0, 1, 2$, as $2^1 = 2$)
Quantities $s_k$ defined by eq. (19) serve as the coefficients in the recurrence formula which according to eq. (25) in the matrix form reads as

$$
T_M = s_1 \cdot T_{M-1} - s_2 \cdot T_{M-2} = (\alpha - \delta) \cdot T_{M-1} + (\alpha \delta - \varphi \alpha) \cdot T_{M-2} \quad M \geq 2;
$$

by equating the corresponding matrix elements on the left and the right side, one obtains

- $A_M = (\alpha - \delta) \cdot A_{M-1} + (\alpha \delta - \varphi \alpha) \cdot A_{M-2}$  
  \hspace{1cm} ($58a$)

- $R_M = (\alpha - \delta) \cdot R_{M-1} + (\alpha \delta - \varphi \alpha) \cdot R_{M-2}$  
  \hspace{1cm} ($58b$)

- $S_M = (\alpha - \delta) \cdot S_{M-1} + (\alpha \delta - \varphi \alpha) \cdot S_{M-2}$  
  \hspace{1cm} ($58c$)

- $D_M = (\alpha - \delta) \cdot D_{M-1} + (\alpha \delta - \varphi \alpha) \cdot D_{M-2}$  
  \hspace{1cm} ($58d$)

The initial conditions (15) are given by eq. (54) and

$$
T_0 = \begin{bmatrix}
A_0 - S_0 \\
R_0 - D_0
\end{bmatrix} = \begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix}
$$

As $l = 1$, $2^l = 2$, and the recurrence formula expresses $A_M$-polynomials in terms of two preceding polynomials, $A_{M-1}$ and $A_{M-2}$, $M \geq 2$. The same is true for the polynomials $R_M$, $S_M$ and $D_M$, with the recurrence formulæ of the same form as the topological consequence of all the fasciagrams $A_M$, $R_M$, $S_M$ and $D_M$, $M \geq 2$, sharing the same inner fragment.

Derivatives $B_M$ and $C_M$ of the fasciagraph $A_M$ are depicted below.
and according to eqs. (35) and (37), one can express the acyclic polynomials of $B_M$ and $C_M$ as

$$B_M = [V - V'] \begin{bmatrix} a - \sigma \\ \theta - \delta \end{bmatrix}^M \begin{bmatrix} U \\ U' \end{bmatrix}$$  \hspace{1cm} (60)$$

and

$$C_M = [V' - V] \begin{bmatrix} a - \sigma \\ \theta - \delta \end{bmatrix}^M \begin{bmatrix} U' \\ U'' \end{bmatrix} = \begin{bmatrix} A_1 - A_1' \\ A_1' - A_1'' \end{bmatrix}^M \begin{bmatrix} U \\ U' \end{bmatrix}$$ \hspace{1cm} (61)$$

Recurrence formulae have the form of eqs. (58)

$$B_M = (a - \delta) \cdot B_{M-1} + (\alpha \delta - \sigma \rho) \cdot B_{M-2}$$ \hspace{1cm} (62)$$

with the initial conditions given by

$$B_0 = V \cdot U - V' \cdot U''$$ \hspace{1cm} (64)$$

As indicated earlier by eq. (29), the application of Heilbronner's formula at the right and the left side of the fasciagraph establishes some relationship between different acyclic polynomials. In the case of fasciagraphs with $l = 1$, eq. (29) reads

$$A_{M+1} = a \cdot A_M - \sigma \cdot R_M$$ \hspace{1cm} (66)$$

and comparison of both formulae gives

$$R_M/S_M = \phi/\sigma$$ for all $M$ \hspace{1cm} (68)$$

Similarly, for the acyclic polynomial of $R_{M+1}$ one obtains

$$R_{M+1} = \phi \cdot A_M - \delta \cdot R_M$$ \hspace{1cm} (69)$$

$$R_{M+1} = a \cdot R_M - \sigma \cdot D_M$$ \hspace{1cm} (70)$$

and comparison gives

$$A_M + D_M = \frac{\alpha + \delta}{\rho} \text{ for all } M$$ \hspace{1cm} (71)$$

In a completely analogous manner, one has

$$S_{M+1} = a \cdot S_M - \sigma \cdot D_M$$ \hspace{1cm} (72)$$

$$S_{M+1} = \sigma \cdot A_M - \delta \cdot S_M$$ \hspace{1cm} (73)$$
and
\[ D_{M+1} = \varphi \cdot S_M - \delta \cdot D_M \quad (74) \]
\[ D_{M+1} = \sigma \cdot R_M - \delta \cdot D_M \quad (75) \]
where comparison reproduces eqs. (68) and (71). Combining eqs. (66) and (69), both containing $A$- and $R$-polynomials, one reproduces the recurrence formulae (58a) and (58b) for $A_M$- and $R_M$-polynomials. Similarly, combining eqs. (72) and (74), both containing $S$- and $D$-polynomials, one reproduces the recurrence formulae (58c) and (58d) for polynomials $S_M$ and $D_M$.

From eqs. (66)—(75), one is able to express $A_M$ and $D_M$ in terms of two $R_M$'s or $S_M$'s as well as $R_M$ and $S_M$ in terms of two $A_M$'s and $D_M$'s. For example, one has
\[ \varphi A_M = R_{M+1} + \delta \cdot R_M \quad (76) \]
\[ \sigma R_M = D_{M+1} + \delta \cdot D_M \quad (77) \]
and its immediate consequence
\[ (\varphi \sigma) A_M = D_{M+2} + 2 \delta D_{M+1} + \delta^2 D_M \quad (78) \]

Similarly, $R_M$, $S_M$ and $D_M$ can be expressed in terms of three $S_M$'s, $R_M$'s and $A_M$'s, respectively.

Eq. (68) serves as a definition of new polynomials $Q_M$
\[ R_M = \varphi Q_M, \quad S_M = \sigma Q_M \quad (79) \]
and comparison with eq. (71) clarifies their meaning as
\[ Q_M = \frac{R_M}{\varphi} = \frac{A_M + D_M}{\alpha + \delta} \quad (80) \]
with the initial conditions being
\[ Q_0 = 0; \quad Q_1 = 1 \quad (81) \]

As $Q_M$ is a combination of $A_M$- and $D_M$-polynomial, which obey the same recurrence formula, eq. (58), it has also to satisfy that recurrence formula, namely
\[ Q_M = (\alpha - \delta) Q_{M-1} + (\alpha \delta - \varphi \sigma) Q_{M-2} \quad (82) \]

Because of eq. (79), it is easy to express $R_M$ and $S_M$ when $Q_M$-polynomials are given. Polynomials $A_M$ and $D_M$ are also simply related to them.

The explicit expressions in terms of $\alpha$, $\varphi$, $\sigma$ and $\delta$ for polynomials $Q_M$ and acyclic polynomials of $A_M$, $R_M$, $S_M$ and $D_M$ up to $M = 6$ are given in Appendix 1.

Comparing $A_M$ with $-D_M$ one recognizes that when $A_M$ is defined quite generally as a polynomial in $\alpha$ and $\delta$,
\[ A_M = P_M (\alpha, \delta) \quad (83) \]
then one has the relationship
\[ D_M = -P_M (-\delta, -\alpha). \quad (84) \]

Further, one should verify that $A_M$ and $D_M$ may be defined by $M \times M$ determinants of the form
Eqn. (87) exhibits implicitly the relationship (84). Expanding $A_M$ or $D_M$ over the first row of the corresponding determinant and comparing with the eqs. (66), (67), (74), (75), and (79) one obtains also determinants defining $Q_M$. According to eqs. (83) and (84) the two determinants are obviously related as follows

$$Q_M(a, \delta) = -Q_M(-\delta, -a).$$

From Appendix 1 one immediately realizes the regularities in the structure of coefficients and the point will be illustrated on the example of $A_M$-polynomials.

$A_M$-polynomial can be written as

$$A_M = \sum_{\lambda=0}^{[M/2]} (-1)^\lambda \xi^\lambda \cdot f(M, \lambda) (a, \delta)$$

where $f(M, \lambda) (a, \delta)$ is a polynomial in $a$ and $\delta$ of the degree $(M - 21)$

$$f(M, \lambda) (a, \delta) = \sum_{j=0}^{M-2\lambda} \alpha_j (M, \lambda) a^{M-2\lambda-j} \delta^j$$
Reccurrence formula (58a) for the $A_M$'s results in a recursion for the $f^{(M,\lambda)}$'s
\begin{equation}
f^{(M,\lambda)} = f^{(M-2,\lambda-1)} + (a\delta) f^{(M-2,\lambda)} + (a - \delta) f^{(M-1,\lambda)}
\end{equation}
and consequently in a recursion for the $a_j^{(M,\lambda)}$-coefficients
\begin{equation}
a_j^{(M,\lambda)} = a_j^{(M-2,\lambda-1)} + a_{j-1}^{(M-1,\lambda)} - a_{j-1}^{(M-1,\lambda)} + a_j^{(M-1,\lambda)}
\end{equation}
j = 0, 1, \ldots, \lambda; \quad \lambda = 0, 1, \ldots, [M/2]

One has $f^{(M,0)} (\alpha, \delta) = \alpha^M$ (this corresponds to deleting all linking bonds without their incident vertices in $A_M$) and therefore
\begin{equation}
a_0^{(M,0)} = 1
\end{equation}
The above condition determines the coefficients as
\begin{equation}
a_j^{(M,\lambda)} = (-1)^j \left( \begin{array}{c} M - \lambda - j \\ \lambda \\
\end{array} \right) \left( \begin{array}{c} \lambda + j - 1 \\ \lambda - 1 \\
\end{array} \right)
\end{equation}
and the $A_M$-polynomials of fasciagraph with $l = 1$ are explicitly given in terms of $\alpha$, $\delta$, $\sigma$ and $\delta$ as follows
\begin{equation}
A_M = \alpha^M + \sum_{\lambda=1}^{[M/2]} (-1)^\lambda (\sigma \delta)^\lambda \sum_{j=0}^{M-2\lambda} (-1)^j \left( \begin{array}{c} M - \lambda - j \\ \lambda \\
\end{array} \right) \left( \begin{array}{c} \lambda + j - 1 \\ \lambda - 1 \\
\end{array} \right)
\end{equation}
The polynomials $A_M$, namely their related coefficients $a_j^{(M,\lambda)}$, $j = 0, 1, \ldots, \lambda; \quad \lambda = 0, 1, \ldots, [M/2]$, are listed in Appendix 2. for $M = 7, 8, \ldots, 20$.

Because of
\begin{equation}
\sum_{j=0}^\lambda |a_j^{(M,\lambda)}| = \sum_{j=0}^\lambda \left( \begin{array}{c} M - \lambda - j \\ \lambda \\
\end{array} \right) \left( \begin{array}{c} \lambda + j - 1 \\ \lambda - 1 \\
\end{array} \right) = \left( \begin{array}{c} M \\ 2\lambda \\
\end{array} \right)
\end{equation}
there are altogether $\left( \begin{array}{c} M \\ 2\lambda \\
\end{array} \right)$ contributions containing $(\sigma \delta)^\lambda$ term as the result of application of Heilbronner's formula to all edges of $A_M$. The total number of contributions to polynomial $A_M$ is
\begin{equation}
\sum_{\lambda=0}^{[M/2]} \left( \begin{array}{c} M \\ 2\lambda \\
\end{array} \right) = 2^{M-1}
\end{equation}
as the number of linking bonds in fasciagraph $A_M$ is $(M - 1)$ and Heilbronner's-like formula (4) gives two contributions per each bond.

Let us now proceed to study the characteristic polynomials $\bar{A}_M$, $\bar{R}_M$, $\bar{S}_M$ and $\bar{D}_M$, $\bar{B}_M$ and $\bar{C}_M$ of the fasciagraph $A_M$ and its derivatives $B_M$ and $C_M$. As here $l = 1$, no difficulties with the deletion of cycles appear and all the formu-
lae derived in the present chapter and the expressions listed in Appendix 1. and Appendix 2. are valid also for $A_M$, $R_M$, $S_M$, $D_M$, $B_M$ and $C_M$ after the appropriate change of acyclic polynomials ($a$, $q$, $o$, $d$, etc.) by their corresponding characteristic polynomials ($a$, $q$, $o$, $d$, etc.).

7. THE ACYCLIC AND THE CHARACTERISTIC POLYNOMIAL OF A ROTAGRAPHD WITH $1 = 1$

First, we will study the acyclic polynomial of the rotagraph $U_M$ and its derivative $V_M$ (depicted below).

According to eqs. (42) and (47) polynomials $U_M$ and $V_M$ can be expressed as

$$U_M = \text{tr} T_M = \text{tr} \left[ \begin{array}{cc} a & -\sigma \\ \phi & -\delta \end{array} \right]^M$$

(100)

and

$$V_M = \text{tr} (T_{M-2} W') = \text{tr} \left( \begin{array}{cc} a & -\sigma \\ \phi & -\delta \end{array} \right)^{M-2} \begin{bmatrix} V' - V' s \\ V' r - V' ts \end{bmatrix}$$

(101)

As $U_M$ and $V_M$ are combinations of polynomials $A_M$, $R_M$, $S_M$ and $D_M$

$$U_M = A_M - D_M$$

(102)

$$V_M = V' \cdot A_{M-2} - V' r \cdot S_{M-2} - V' s \cdot R_{M-2} + V' ts \cdot D_{M-2}$$

(103)

they must satisfy the same recurrence relation as those polynomials which results in

$$U_M = (a - \delta) U_{M-1} + (a \delta - q \phi) U_{M-2}$$

(104)

$M \geq 2$
with the initial conditions being
\[ U_0 = tr I = 2 \]  
\[ V_2 = V' - V'_{rs} \]

We have repeated eqs. (43) and (48) for a special case of rotagraphs with \( l = 1 \).

The explicit expressions for acyclic polynomials of \( U_M \) up to \( M = 6 \) are given in Appendix 3.

Using eq. (78), one can express \( U_M \) in terms of \( D_M \)'s
\[ (q \sigma) U_M = D_{M+2} + 2g \cdot D_{M+1} = (q \sigma - g) \cdot D_M \]  \( (108) \)

or in terms of \( A_M \)'s
\[ (q \sigma) U_M = -A_{M+2} + 2a \cdot A_{M+1} + (q \sigma - a^2) \cdot A_M \]  \( (109) \)

Let us now proceed to study the characteristic polynomial \( \overline{U}_M \) of a rotagraph \( U_M \). When one applies eq. (3) to any linking bond of \( U_M \) one has to delete all cycles containing that bond. As \( l = 1 \), each cycle has to pass over all linking bonds and in each monomer unit \( A_1 = A \) over some path \( P_{sr} \) connecting vertices \( s \) and \( r \). Therefore, one has
\[ \overline{U}_M = \overline{A}_M - \overline{D}_M - 2 \left[ \sum_{P_{sr}} \overline{A}_{P_{sr}} \right] \]
\[ (110) \]

where \( A_{P_{sr}} \) denotes the subgraph obtained by deletion of all the vertices of the path \( P_{sr} \) from \( A \) and the summation goes over all paths \( P_{sr} \) between vertices \( s \) and \( r \) in \( A \).

On the other hand, the use of cyclic symmetry, see eq. (50), gives
\[ \overline{U}_M = \overline{A}_M - \overline{D}_M - 2 \left[ \sum_{P_{sr}} \overline{A}_{P_{sr}} \right] M = \left[ \sum_{j=1}^{M} A(\omega_j) \right] \]
\[ (111) \]

and now the representative graph \( A(\omega_j) \) has the especially simple form

\[ \begin{array}{c}
A_{sr} + \omega j \\
\circ \\
\rightarrow \\
A_{sr} + \omega j \\
\end{array} \]

\[ (A(\omega_j)) \]

The above equation clarifies the meaning of the important topological function \( s_3 = a \delta - q \sigma \) appearing in the recurrence relation for the characteristic polynomial of fasciagraphs with \( l = 1 \). As shown in Appendix 4, eq. (111) applied to rotagraph \( U_M \) with \( M = 2 \) leads to the following identity:
ACYCLIC POLYNOMIAL

\[ \overline{a \delta - \varrho \sigma} = - \left[ \sum_{P_{ar}} A_{P_{ar}} \right]^2 \]  

(112)

namely, \( s_2 \) is always a non-positive quantity. The identity is valid for vertices \( s \) and \( r \) being \( (A_{sr} = 1) \) or not being neighbours \( (A_{sr} = 0) \) in the monomer unit graph \( A \); however, in the former case the edge connecting \( s \) and \( r \) is treated as a path too.

The identity also appeared recently in topological studies of the law of alternating polarity\(^\text{16}\) as a graph-theoretical reinterpretation of an older result\(^\text{17}\).

Acknowledgement. — We would like to express our thanks to Prof. J. N. Silvermann and Dr. B. Weimann for their valuable comments and suggestions. One of us (A. G.) thanks the Max-Planck-Gesellschaft for a grant, the other two (O. E. P., N. N. T.) thank the Deutsche Forschungsmehrschein, Bonn, and the Bulgarian Academy of Science, Sofia, for making the cooperation possible.

REFERENCES

1. O. E. Polansky and N. N. Tyutyulkov, MATCH 3 (1977) 149.

APPENDIX 1

The explicit expressions for \( Q_{M} \)-polynomials and \( A_{M} \)-, \( R_{M} \)-, \( S_{M} \)- and \( D_{M} \)-acyclic polynomials up to \( M = 6 \) are given below.

The same expressions apply for the characteristic polynomials \( \overline{A_{M}} \), \( \overline{R_{M}} \), \( \overline{S_{M}} \) and \( D_{M} \) after the appropriate change of \( a \), \( \varrho \), \( \sigma \) and \( \delta \) by \( \overline{a} \), \( \overline{\varrho} \), \( \overline{\sigma} \) and \( \overline{\delta} \), respectively.

\[ Q_0 = 1 \]
\[ Q_1 = 1 \]
\[
Q_2 = \frac{\alpha^2 - \delta^2}{\alpha + \delta}
\]
\[
Q_3 = \frac{\alpha^2 + \delta^2}{\alpha + \delta} - (\varphi \sigma) \frac{\alpha + \delta}{\alpha + \delta}
\]
\[
Q_4 = \frac{\alpha^2 - \delta^2}{\alpha + \delta} - (\varphi \sigma) \frac{2 \alpha^2 - \delta^2}{\alpha + \delta}
\]
\[
Q_5 = \frac{\alpha^2 + \delta^2}{\alpha + \delta} - (\varphi \sigma) \left( \frac{\alpha^2 + \delta^2 - \alpha \delta}{\alpha + \delta} \right) + (\varphi \sigma)^2
\]
\[
Q_6 = \frac{\alpha^2 - \delta^2}{\alpha + \delta} - (\varphi \sigma) \left( \frac{4 \alpha^2 - \delta^2 - 2 \alpha \delta + \delta^2}{\alpha + \delta} \right) + (\varphi \sigma)^2 \frac{3 \alpha^2 - \delta^2}{\alpha + \delta}
\]
\[A_0 = 1\]
\[A_1 = \alpha\]
\[A_2 = \alpha^2 - \varphi \sigma\]
\[A_3 = \alpha^3 - (\varphi \sigma) (2 \alpha - \delta)\]
\[A_4 = \alpha^4 - (\varphi \sigma) (3 \alpha^2 - 2 \alpha \delta + \delta^2) + (\varphi \sigma)^2\]
\[A_5 = \alpha^5 - (\varphi \sigma) (4 \alpha^3 - 3 \alpha^2 \delta + 2 \alpha \delta^2 - \delta^3) + (\varphi \sigma)^2 (3 \alpha - 2 \delta)\]
\[A_6 = \alpha^6 - (\varphi \sigma) (5 \alpha^4 - 4 \alpha^3 \delta + 3 \alpha^2 \delta^2 - 2 \alpha \delta^3 + \delta^4) + (\varphi \sigma)^2 (6 \alpha^2 - 6 \alpha \delta + 3 \delta^2) - (\varphi \sigma)^3\]
\[R_0 = 0\]
\[R_1 = \varphi\]
\[R_2 = \varphi (\alpha - \delta)\]
\[R_3 = \varphi [(\alpha^2 - \alpha \delta + \delta^2) - (\varphi \sigma)]\]
\[R_4 = \varphi [(\alpha^3 - \alpha^2 \delta + \alpha \delta^2 - \delta^3) - (\varphi \sigma) (2 \alpha - 2 \delta)]\]
\[R_5 = \varphi [(\alpha^4 - \alpha^3 \delta + \alpha^2 \delta^2 - \alpha \delta^3 + \delta^4) - (\varphi \sigma) (3 \alpha^2 - 4 \alpha \delta + 3 \delta^2) + (\varphi \sigma)^2]\]
\[R_6 = \varphi [(\alpha^5 - \alpha^4 \delta + \alpha^3 \delta^2 - \alpha^2 \delta^3 + \alpha \delta^4 - \delta^5) - (\varphi \sigma) (4 \alpha^3 - 6 \alpha^2 \delta + 6 \alpha \delta^2 - 4 \delta^3) + (\varphi \sigma)^2 (3 \alpha - 3 \delta)]\]
\[S_0 = 0\]
\[S_1 = \alpha\]
\[S_2 = \alpha (\alpha - \delta)\]
\[S_3 = \alpha [(\alpha^2 - \alpha \delta + \delta^2) - (\varphi \sigma)]\]
\[S_4 = \alpha [(\alpha^3 - \alpha^2 \delta + \alpha \delta^2 - \delta^3) - (\varphi \sigma) (2 \alpha - 2 \delta)]\]
\[S_5 = \alpha [(\alpha^4 - \alpha^3 \delta + \alpha^2 \delta^2 - \alpha \delta^3 + \delta^4) - (\varphi \sigma) (3 \alpha^2 - 4 \alpha \delta + 3 \delta^2) + (\varphi \sigma)^2]\]
\[S_6 = \alpha [(\alpha^5 - \alpha^4 \delta + \alpha^3 \delta^2 - \alpha^2 \delta^3 + \alpha \delta^4 - \delta^5) - (\varphi \sigma) (4 \alpha^3 - 6 \alpha^2 \delta + 6 \alpha \delta^2 - 4 \delta^3) + (\varphi \sigma)^2 (3 \alpha - 3 \delta)]\]
\[D_0 = 1\]
\[D_1 = \delta\]
\[D_2 = - \delta^2 + (\varphi \sigma)\]
\[D_3 = \delta^2 - (\varphi \sigma) (2 \delta - \alpha)\]
\[D_4 = - \delta^4 + (\varphi \sigma) (3 \delta^2 - 2 \alpha \delta + \alpha^2) - (\varphi \sigma)^2\]
\[D_5 = \delta^5 - (\varphi \sigma) (4 \delta^3 - 3 \delta^2 \alpha + 2 \delta \alpha^2 - \delta^3) + (\varphi \sigma)^2 (3 \delta - 2 \alpha)\]
\[D_6 = - \delta^6 + (\varphi \sigma) (5 \delta^4 - 4 \delta^3 \alpha + 3 \delta^2 \alpha^2 - 2 \delta \alpha^3 + \alpha^3) - (\varphi \sigma)^2 (6 \delta^2 - 6 \delta \alpha + 3 \alpha^2) + (\varphi \sigma)^3\]
APPENDIX 2.

The Coefficients $a_j^{(m,i)}$, $j = 0, 1, \ldots l$; $l = 0, 1, \ldots [M/2]$ are listed below for $M = 7, 8, \ldots, 20$.

For $l = 0, 1$, the table is as follows:

| $M$ | $j$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
|-----|-----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 7   | 1   | 6 | -5| 4 | -3| 2 | -1|   |   |   |   |   |   |   |   |   |   |   |   |
| 8   | 1   | 7 | -6| 5 | -4| 3 | -2| 1 |   |   |   |   |   |   |   |   |   |   |   |   |
| 9   | 1   | 8 | -7| 6 | -5| 4 | -3| 2 | -1|   |   |   |   |   |   |   |   |   |   |   |
| 10  | 1   | 9 | -8| 7 | -6| 5 | -4| 3 | -2| 1 |   |   |   |   |   |   |   |   |   |   |
| 11  | 1   | 10| -9| 8 | -7| 6 | -5| 4 | -3| 2 | -1|   |   |   |   |   |   |   |   |   |
| 12  | 1   | 11| -10| 9 | -8| 7 | -6| 5 | -4| 3 | -2| 1 |   |   |   |   |   |   |   |   |
| 13  | 1   | 12| -11| 10| -9| 8 | -7| 6 | -5| 4 | -3| 2 | 1 |   |   |   |   |   |   |   |
| 14  | 1   | 13| -12| 11| -10| 9 | -8| 7 | -6| 5 | -4| 3 | -2| 1 |   |   |   |   |   |   |
| 15  | 1   | 14| -13| 12| -11| 10| -9| 8 | -7| 6 | -5| 4 | -3| 2 | -1|   |   |   |   |   |
| 16  | 1   | 15| -14| 13| -12| 11| -10| 9 | -8| 7 | -6| 5 | -4| 3 | -2| 1 |   |   |   |   |
| 17  | 1   | 16| -15| 14| -13| 12| -11| 10| -9| 8 | -7| 6 | -5| 4 | -3| 2 | -1|   |   |   |
| 18  | 1   | 17| -16| 15| -14| 13| -12| 11| -10| 9 | -8| 7 | -6| 5 | -4| 3 | -2| 1 |   |   |
| 19  | 1   | 18| -17| 16| -15| 14| -13| 12| -11| 10| -9| 8 | -7| 6 | -5| 4 | -3| 2 | -1|   |
| 20  | 1   | 19| -18| 17| -16| 15| -14| 13| -12| 11| -10| 9 | -8| 7 | -6| 5 | -4| 3 | -2| 1 |
### $l = 2$

| $j$ | $M$ | 0   | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 17 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 7   | 10  | -12 | 9   | -4  |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 8   | 15  | -20 | 18  | -12 | 5   |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 9   | 21  | -30 | 30  | -24 | 15  | -6  |     |     |     |     |     |     |     |     |     |     |     |     |
| 10  | 28  | -42 | 45  | -40 | 30  | -18 | 7   |     |     |     |     |     |     |     |     |     |     |     |
| 11  | 36  | -56 | 63  | -60 | 50  | -36 | 21  | -8  |     |     |     |     |     |     |     |     |     |     |
| 12  | 45  | -72 | 84  | -84 | 75  | -60 | 42  | -24 | 9   |     |     |     |     |     |     |     |     |     |
| 13  | 55  | -90 | 108 | -112| 105 | -90 | 70  | -48 | 27  | -10 |     |     |     |     |     |     |     |     |
| 14  | 66  | -110| 135 | -144| 140 | -126| 105 | -80 | 54  | -30 | 11  |     |     |     |     |     |     |     |
| 15  | 78  | -132| 165 | -180| 180 | -168| 147 | -120| 90  | -60 | 33  | -12 |     |     |     |     |     |     |
| 16  | 91  | -156| 198 | -220| 225 | -216| 196 | -168| 135 | -100| 66  | -36 | 13  |     |     |     |     |     |
| 17  | 105 | -182| 234 | -264| 275 | -270| 252 | -224| 189 | -150| 110 | -72 | 39  | -14 |     |     |     |     |
| 19  | 136 | -240| 315 | -364| 390 | -396| 385 | -360| 324 | -280| 231 | -180| 130 | -84 | 45  | -16 |     |     |
| 20  | 153 | -272| 360 | -420| 455 | -468| 462 | -440| 405 | -360| 308 | -252| 195 | -140| 90  | -48 | 17  |

### $l = 3$

| $j$ | $M$ | 0   | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 17 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 7   | 4   | -3  |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 8   | 10  | -12 | 6   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 9   | 20  | -30 | 24  | -10 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 10  | 35  | -60 | 60  | -40 | 15  |     |     |     |     |     |     |     |     |     |     |     |     |     |
| 11  | 56  | -105| 120 | -100| 60  | -21 |     |     |     |     |     |     |     |     |     |     |     |     |
| 12  | 84  | -168| 210 | -206| 150 | -84 | 28  |     |     |     |     |     |     |     |     |     |     |     |
| 13  | 120 | -252| 336 | -336| 300 | -210| 112 | -36 |     |     |     |     |     |     |     |     |     |     |
| 14  | 165 | -360| 504 | -560| 525 | -420| 280 | -144| 45  |     |     |     |     |     |     |     |     |     |
| 15  | 220 | -495| 720 | -840| 840 | -735| 560 | -360| 180 | -55 |     |     |     |     |     |     |     |     |
| 16  | 286 | -660| 990 | -1200|1260| -1176|980 | -720| 450 | -220| 66  |     |     |     |     |     |     |     |
| 17  | 364 | -858| 1320| -1650|1800| -1764|1568| -1260|900 | -550| 264 | -78 |     |     |     |     |     |     |
| 18  | 455 | -1092|1710| -2200|2475| -2520|2352| -2018|1575| -1100|660 | -312| 91  |     |     |     |     |     |
| 19  | 560 | -1365|2184| -2860|3300| -3465|3360| -3024|2520| -1925|1320| -780| 364 | -105|     |     |     |     |
| 20  | 680 | -1680|2730| -3640|4290| -4620|4620| -4320|3780| -3080|2310| -1580|910 | -420| 120 |     |     |     |
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APPENDIX 3.

The explicit expressions in terms of \(a\), \(q\), \(e\) and \(b\) polynomial for \(U_M\) acyclic polynomials up to \(M = 6\) are given below.

\[
\begin{align*}
U_0 &= 2 \\
U_1 &= a - \delta \\
U_2 &= (a^2 + \delta^2) - 2 (q \sigma) \\
U_3 &= (a^2 - \delta^2) - 3 (q \sigma) (a - \delta) \\
U_4 &= (a^4 + \delta^4) - 4 (q \sigma) (a^2 - \alpha \delta + \delta^2) + 2 (q \sigma)^2 \\
U_5 &= (a^2 - \delta^2) - 5 (q \sigma) (a^2 - a \delta^2 + \alpha \delta^2 + \delta^2) + 5 (q \sigma)^2 (a - \delta) \\
U_6 &= (a^4 + \delta^4) - 6 (q \sigma) (a^4 - a^3 \delta + a^2 \delta^2 - a^3 \delta^2 + a \delta^4 + \delta^4) + (q \sigma)^2 (9 a^2 - 12 a \delta + 9 \delta^2) - 2 (q \sigma)^3
\end{align*}
\]

APPENDIX 4.

An Important Topological Identity

Let us consider the rotagraph \(U_M\) with \(M = 2\). Then, \(\omega_1 = -1\), \(\omega_2 = +1\), and eq. (111) reads as

\[
a^2 - 2q \sigma + \delta^2 - 2 \left[ \sum_{P_{sr}} \bar{A}_{P_{sr}} \right]^2 = A (\omega_1 = -1) \cdot A (\omega_2 = +1) \tag{4.1}
\]

where the representative graphs \(A (\omega_1 = -1)\) and \(A (\omega_2 = +1)\) are depicted below for the case of vertices \(s\) and \(r\) not being neighbours in the original graph \(A\).

\[
\begin{align*}
(A) & \quad (A(\omega_1)) \\
\begin{array}{c}
\circ \\
\text{s} \\
\circ
\end{array} & \quad \begin{array}{c}
-1 \\
\circ \\
\text{s} \\
\circ \\
\text{r}
\end{array}
\end{align*}
\]

Applying eq. (3) for \(A (\omega_1)\) and \(A (\omega_2)\) one has

\[
\begin{align*}
A (\omega_1) &= a - \delta + 2 \left[ \sum_{P_{sr}} \bar{A}_{P_{sr}} \right] \tag{4.2a} \\
\bar{A} (\omega_2) &= a - \delta - 2 \left[ \sum_{P_{sr}} \bar{A}_{P_{sr}} \right] \tag{4.2b}
\end{align*}
\]

Note the change of sign in the third term of eq. (3.2a) as the result of the presence of an edge with the weight \((-1)\). From eqs. (4.1)–(4.2) it follows

\[
\bar{a} \cdot \delta - \bar{\sigma} \cdot \sigma = - \left[ \sum_{P_{sr}} \bar{A}_{P_{sr}} \right]^2 \tag{4.3}
\]

Let us now consider the case of vertices \(s\) and \(r\) being neighbours in the monomer graph. This is denoted by \(A^*\) and depicted below
<table>
<thead>
<tr>
<th>$j$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M$</td>
<td>$l=7$</td>
<td>$l=8$</td>
<td>$l=9$</td>
<td>$l=10$</td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
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<td>8</td>
<td>-7</td>
<td></td>
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<td></td>
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<td></td>
</tr>
<tr>
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<td>36</td>
<td>-56</td>
<td>28</td>
<td>-84</td>
<td>1</td>
<td>-8</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>120</td>
<td>-252</td>
<td>224</td>
<td>-84</td>
<td>165</td>
<td>-360</td>
<td>324</td>
<td>-120</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>330</td>
<td>-840</td>
<td>1008</td>
<td>-672</td>
<td>210</td>
<td>45</td>
<td>-72</td>
<td>36</td>
<td>-120</td>
<td>10</td>
<td>-9</td>
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<td>330</td>
<td>55</td>
<td>-90</td>
<td>45</td>
<td>1</td>
</tr>
</tbody>
</table>
It is obvious that

\[ \bar{\sigma} = \bar{\sigma}; \bar{\delta} = \bar{\delta} \]

and

\[ \sum_{P_{sr}} A' P_{sr} = \bar{\sigma} + \sum_{P_{sr}} \bar{A}' P_{sr} \]

as the edge connecting \( s \) and \( r \) is a path in \( A' \) but not in \( A \).

Application of eq. (3) gives

\[ \bar{a}' = a_0 - 2 \left[ \sum_{P_{sr}} \bar{A}' P_{sr} \right] \]

By use of eqs. (4.4)-(4.6), eq. (4.3) can be rewritten as follows

\[ \bar{a}' \cdot \bar{\delta}' - \bar{\sigma}' \cdot \bar{\sigma}' = - \left[ \sum_{P_{sr}} A' P_{sr} \right] \]

Therefore, the same identity is valid regardless of connectivity of vertices \( s \) and \( r \) in the monomer graph.

SAZETAK

Aciklički i karakteristični polinom regularnih konjugiranih polimera i njihovih derivata

A. Graovac, O. E. Polansky i N. N. Tyutyulkov

Opisan je postupak za studij acikličkog i karakterističnog polinoma regularnih konjugiranih polimera.

Za regularni polimer sa 1 veza među monomernim jedinicama prvo se konstruira \( 2' \times 2' \) polinomska matrica \( T_1 \). Njeni matrični elementi predstavljaju aciklički polinom monomernog grafa, te njegovih podgrafova dobivenih uzastopnim uklanjanjem atoma koji služe kao vezna mjesta. Aciklički polinom fascigrafa (koji predstavlja polimer sa otvorenim krajevima) i nekih njegovih podgrafova dobijaju se kao odgovarajući matrični elementi matrice \( T_1 \), gdje \( M \) označava stupanj polimerizacije promatranog polimera. Aciklički polinom rotagrafa (koji predstavlja polimer zatvoren na samom sebi) jednak je tragu matrice \( T_1 \).

Dokazano je da aciklički polinomi regularnog polimera i nekih njegovih derivata zadovoljavaju jednu te istu rekurentnu relaciju koja sadrži \( 2' + 1 \) članova. Koefficijenti koji ulaze u rekurziju su izvedeni samo iz poznavanja matrice \( T_1 \), te su stoga neovisni o \( M \).

Dokazano je da karakteristični polinom regularnog polimera postupak analogan formalizmu matrice \( T_1 \) smo proveli samo za poseban slučaj \( l = 1 \) pri čemu se dobiva jedna već poznata rekurentna relacija.

Ipak, u ovom posebnom slučaju uspostavili smo jedan novi prikaz karakterističnog polinoma polimera pomoću determinanti, te ga izričito izrazili preko karakterističnog polinoma monomernog grafa i njegovih podgrafova.