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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 $2^l X 2^l$ 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-

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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.

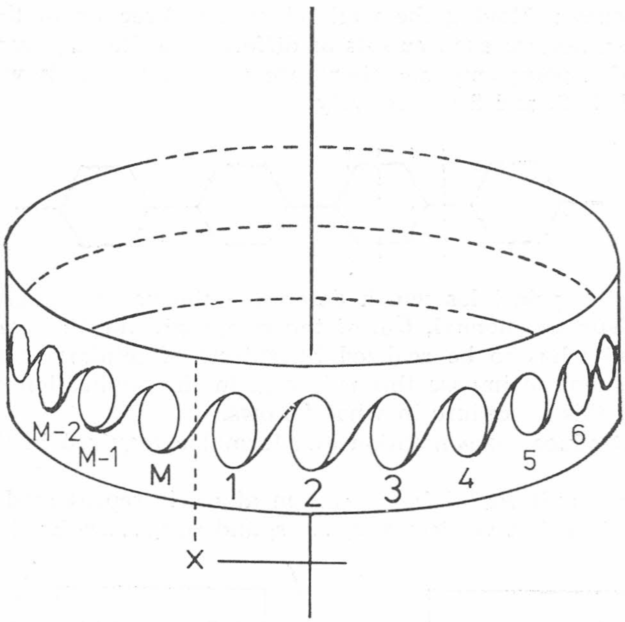
Due to the size of polymers, it is usually quite troublesome to derive their corresponding characteristic and acyclic polynomials if one starts from the basic definitions of these polynomials. In the past, the transfer matrix method (TMM)[3] was used to derive the characteristic polynomial for various polymers.[4] Another approach, mainly based on group theory, is offered in ref. 1. Recently, Kaulgud and Chitgopkar[5] 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 polymers[6] and the total pi-electron energy of polyene chain and its derivatives.[7]. Although the PMM 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 PMM approach is generalized for any number of linking bonds l 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 PMM 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 defined[1] 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 $M \rightarrow \infty$, the description of the polymer by U_M concides with that frequently used in solid



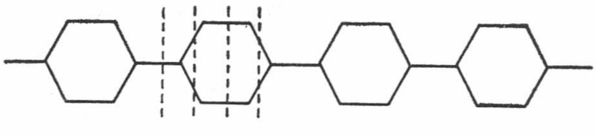
state physics for one-dimensional crystals. Using a similar formalism as there, one may factorize the characteristic polynomial of U_M into exactly M factors,[1] each of them of the degree n where n stands for the number of vertices of the monomeric unit. The fasciagraph, A_M, is obtained from U_M by 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 rotapolymeric polyacene may be understood as being constructed from cisoid or transoid C_4H_2-units, as shown below but the

fasciagraphs 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.

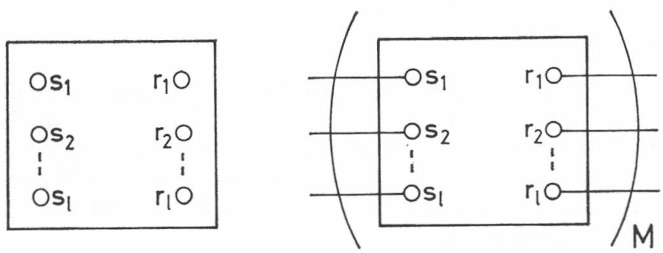
The edges which link two neighbouring monomeric units together cross the walls of the unit cells (see above). They may be understood as the members of a distinct cutset. Moving the walls along the direction of the propagation of the polymer, several such cutsets of different cardinality may be obtained.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



According to the principles which determine the general analytical form of the characteristic polynomial, $\bar{U}_M$, 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



(A_1) (P_M)

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_j and r_j generates a set, e. g. $\{s_j^{\varkappa} \mid 1 \leq \varkappa \leq M\}$. When no danger of confusion appears the index $\varkappa$ is omitted.

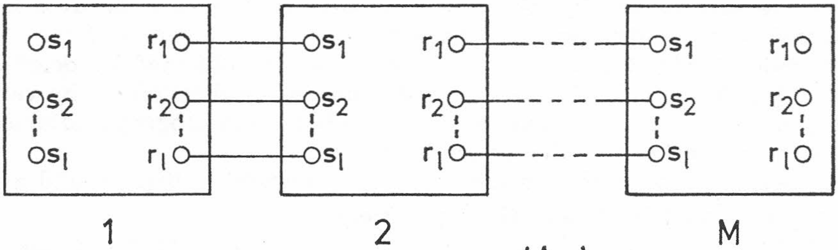
The characteristic polynomial $\Phi(G, \lambda)$ of graph G with n vertices is defined as

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

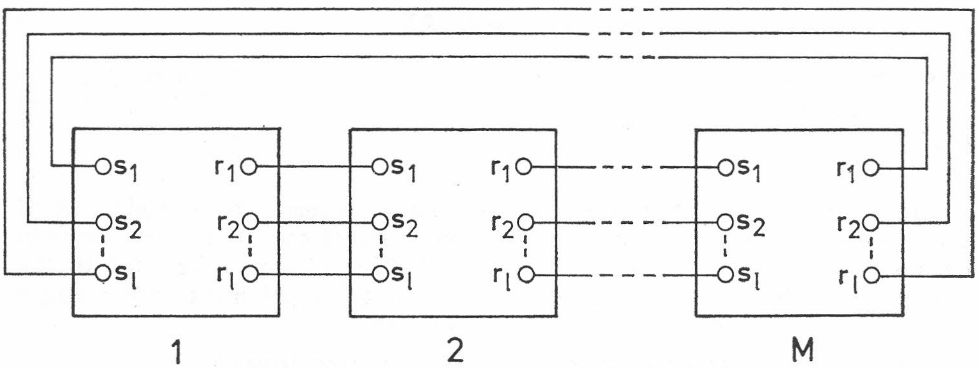
where A is the adjacency matrix of graph G and I stands for the unit matrix. The roots of $\Phi(G, \lambda)$ define the spectrum of G, namely the Hückel molecular orbital energies of the conjugated system represented by G. Using the expansion theorem of determinants, one may express $\Phi(G, \lambda)$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

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

where $D_{ii} = (\lambda I - A)_{ii}$, $\hat{P}$ 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.



(A_M)



(U_M)

The acyclic or matching polynomial $\alpha(G, \lambda)$ of graph G with n vertices is defined by

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

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. (1a), 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 $\alpha(G, \lambda)$ 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

$$\alpha(G, \lambda) = \mu(G, \lambda;\ t = 0)$$

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

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 indicent edges) from G, $G^{(pq)}$ 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

$$\overline{G} = \overline{G^{(pq)}} - \overline{G^{pq}} - 2 \sum_{\alpha} \overline{G^{Z}}\, \alpha \tag{3}$$

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]

$$G = G^{(pq)} - G^{pq} \tag{4}$$

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 FASCIAGRAPH

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 $\binom{l}{0}$ of the terms no edge together with its incident vertices is deleted, in $\binom{l}{1}$ of them one edge together with its incident vertices is deleted, generally, in $\binom{l}{k}$ terms k edges together with their incident vertices are deleted. As the result, one has

$$A_M = A_1 A_{M-1} - \sum_{1 \leq j_1 \leq l} A_1^{s_{j_1}} A_{M-1}^{r_{j_1}} + \sum_{1 \leq j_1 < j_2 \leq l} A_1^{s_{j_1} s_{j_2}} A_{M-1}^{r_{j_1} r_{j_2}} - \ldots +$$

$$+ (-1)^k \sum_{1 \leq j_1 < j_2 < \cdots < j_k \leq l} A_1^{s_{j_1} s_{j_2} \cdots s_{j_k}} A_{M-1}^{r_{j_1} r_{j_2} \cdots r_{j_k}} + \ldots + (-1)^l A_1^{s_1 s_2 \ldots s_l}$$

$$A_{M-1}^{r_1 r_2 \ldots r_l} \tag{5}$$

A_M is expressed as a combination of N acyclic polynomials $A_{M-1}, A_{M-1}^{r_1}, \ldots, A_{M-1}^{r_1 r_2}, \ldots, A_{M-1}^{r_1 r_2 \cdots r_l}$ with the coefficients being the acyclic polynomials of the monomer unit graph and some of its subgraphs, $A_1, A_1^{s_1}, \ldots, A_1^{s_1 s_2}, \ldots, A_1^{s_1 s_2 \cdots s_l}$, respectively.

The recursion formula (4) could be applied to any one of the N acyclic polynomials $A_M, A_M^{r_1}, \ldots, A_M^{r_1 r_2}, \ldots, A_M^{r_1 r_2 \cdots r_l}$, as well, where the r_j's are deleted from the M-th unit. Generally, one has

$$A_M^{r_{i_1} r_{i_2} \cdots r_{i_m}} = A_1^{r_{i_1} r_{i_2} \cdots r_{i_m}} A_{M-1} - \sum_{1 \le j_1 \le l} A_1^{r_{i_1} r_{i_2} \cdots r_{i_m} s_{j_1}} A_{M-1}^{r_{j_1}} + \ldots +$$

$$+ (-1)^k \sum_{1 \le j_1 < j_2 < \cdots < j_k \le l} A_1^{r_{i_1} r_{i_2} \cdots r_{i_m} s_{j_1} s_{j_2} \cdots s_{j_k}} A_{m-1}^{r_{j_1} r_{j_2} \cdots r_{j_k}} +$$

$$+ (-1)^l A_1^{r_{i_1} r_{i_2} \cdots r_{i_m} s_1 s_2 \cdots s_l} A_{M-1}^{r_1 r_2 \cdots r_l} \tag{6}$$

and, as before, any of $A_M^{r_{i_1} r_{i_2} \cdots r_{i_m}}$ is expressed as a combination of the same N acyclic polynomials $A_{M-1}, A_{M-1}^{r_1}, \ldots, A_{M-1}^{r_1 r_2}, \ldots, A_{M-1}^{r_1 r_2 \cdots r_l}$ 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 $A_M^{s_1}, \ldots, A_M^{s_1 s_2}, \ldots$, 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:

$$P(I) = \{\Phi, \{1\}, \ldots, \{1, 2\}, \ldots, \{1, 2, 3\}, \ldots, I\} = \{J \mid J \subseteq I\} = \{I_k \mid 1 \le k \le N\} \tag{7a}$$

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

$$P(R) = \{r_J \mid J \subseteq I\} = \{\varrho k \mid 1 \le k \le N\}, \quad r_J = \{r_j \mid j \varepsilon J\}$$
$$P(S) = \{s_J \mid J \subseteq I\} = \{\sigma k \mid 1 \le k \le N\}, \quad s_J = \{s_j \mid j \varepsilon J\} \tag{7b}$$

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 $I_k \leftrightarrow \varrho_k$, $I_k \leftrightarrow \sigma_k$. Then $\varrho_1 = \sigma_1 = \Phi$, etc.; the cardinalities of the subsets I_k, ϱ_k, and σ_k equal each other $|I_k| = |\varrho_k| = |\sigma_k|$. When all the vertices of ϱ_i and σ_j are deleted from graph G, a subgraph $G^{\sigma_i \varrho_j}$ is obtained. Its acyclic polynomials are denoted by the same symbol as there is no danger of confusion. Since ϱ_1 and σ_1 denote empty sets, we have $G^{\varrho_1 \sigma_1} = G$, $G^{\varrho_1 \sigma_1} = G^{\varrho_1}$ and $G^{\varrho_1 \sigma_1} = G^{\sigma_1}$.

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

$$[A_M^{\varrho_1}, A_M^{\varrho_2}, \ldots, A_M^{\varrho_N}]^t = T_1 [A_{M-1}^{\varrho_1}, A_{\varrho_2}, \ldots, A_{\varrho_N M-1} \tag{8}$$

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

$$(T_1)_{ij} = (-1)^{|\sigma_j|} A_1^{\rho_1 \sigma_j} \tag{9}$$

Applying eq. (8) to the vector $[A_{M-1}^{\varrho_1}, \ldots,]^t$ one obtains

$$[A_M^{\rho_1}, \ldots]^t = T_1^2 [A_{M-2}^{\rho_1}, \ldots]^t$$

Therefore, eq. (8) applied M times gives

$$[A_M^{\rho_1}, A_M^{\rho_2}, \ldots, A_M^{\rho N}]^t = T_1^M [A_0^{\rho_1}, A_0^{\rho_2}, \ldots, A_0^{\rho N}]^t \tag{10}$$

where the elements $A_0^{\varrho_1}, \ldots,$ are, obviously, the numbers.

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

$$A_0 = A_0^{\rho_1} = 1,\ A_0^{\rho_2} = \ldots = A_0^{\rho N} = 0 \tag{11}$$

and eq. (10) becomes

$$[A_M^{\rho_1}, A_M^{\rho_2}, \ldots, A_M^{\rho N}]^t = T_1^M [1, 0, \ldots, 0] \tag{12}$$

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

$$A_M^{\rho\, i \sigma\, j} = \sum_{k=1}^{N} (-1)^{|\sigma\, k|} A_1^{\rho\, i \sigma\, k} A_{M-1}^{\rho\, k \sigma\, j};\ i = 1, 2, \ldots, N \tag{13}$$

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

$$(-1)^{|\sigma_j|} A_0^{\varrho_1 \sigma_j} = \delta_{ij}, \tag{14}$$

hence,

$$T_0 = I. \tag{15}$$

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:

$$T_M = T_1^M, \tag{16}$$

where the $N \times N$ polynomial matrix T_M is given by

$$(T_M)_{ij} = (-1)^{|\sigma_j|} A_M^{\varrho_1 \sigma_j} \tag{17}$$

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 $A_M^{\varrho_1 \sigma_j}$ to the polynomials $A_L^{\varrho_1 \sigma_j}$, $L = M - 1, M - 2, \ldots, 0$, 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:

$$T_1\begin{pmatrix} i_1 i_2 \ldots i_k \\ j_1 j_2 \ldots j_k \end{pmatrix} = \begin{vmatrix} T_{i_1 j_1} & T_{i_1 j_2} & \ldots T_{i_1 j_k} \\ T_{i_2 j_1} & T_{i_2 j_2} & \ldots T_{i_2 j_k} \\ T_{i_k j_1} & T_{i_k j_2} & \ldots T_{i_k j_k} \end{vmatrix} \tag{18}$$

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

$$s_k = \sum_{1\leq j_1<j_2<\cdots<j_k\leq N} T_1\begin{pmatrix} j_1 j_2 \ldots j_k \\ j_1 j_2 \ldots j_k \end{pmatrix} \tag{19}$$

e. g.:

$$s_1 = \mathrm{tr}\, T_1,\ s_2 = \sum_{\substack{i,\, j=1 \\ i<j}}^{N} \begin{vmatrix} T_{ii} & T_{ij} \\ T_{ji} & T_{ii} \end{vmatrix},\ \text{etc.} \tag{20}$$

where tr$A$ denotes the trace of the matrix A.

By definition there is

$$s_0 = 1 \tag{21}$$

As it is known from linear alg( )ra, one can write $\Phi\,(T_1, \lambda)$ as[13a]

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

Applying the Cayley-Hamilton theorem,[13b]

$$\Phi\,(T_1, T_1) = 0 \tag{23}$$

one obtains

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

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

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

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

$$\sum_{k=0}^{N} (-1)^k\, s_k\, A_{N-k}^{\varrho_1\sigma_j} = 0,\ i = 1, 2, \ldots, N,\ j = 1, 2, \ldots, N \tag{26}$$

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 $A_N^{\varrho_1\sigma_j}$ of the N th order is given by recursion containing acyclic polynomials $A_L^{\varrho_1\sigma_j}$ 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 ϱ_1 and σ_j and therefore all the polynomials $A_N^{\varrho_i\sigma_j}$, $i = 1, 2, \ldots, N$, $j = 1, 2, \ldots, N$, obey the recursion formula of the same form. The result can be understood as the topological consequence of the fact that all the polymers $A_N^{\varrho_i\sigma_j}$ share the common inner fragment, namenly 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

$$\sum_{k=0}^{N} (-1)^k s_k A_{M-k}^{\varrho_i\sigma_j} = 0, \; M \geq N \tag{27}$$

In such a way $A_M^{\varrho_i\sigma_j}$, $M \geq N$ is expressed by $A_{M-1}^{\varrho_i\sigma_j}, \ldots, A_{M-N}^{\varrho_i\sigma_j}$ in the same form as is $A_N^{\varrho_i\sigma_j}$ in terms of $A_{N-1}^{\varrho_i\sigma_j}, \ldots, A_0^{\varrho_i\sigma_j}$. 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 $A_M^{\varrho_i\sigma_j}$, $M \geq N$ in terms of a new recursion containing only $A_{N-1}^{\varrho_i\sigma_j}$, $A_{N-2}^{\varrho_i\sigma_j}, \ldots, A_0^{\varrho_i\sigma_j}$. This point of view, however, is of no interest in our further considerations.

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

$$T_M = T_1 \cdot T_{M-1} = T_{M-1} \cdot T_1 \tag{28}$$

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

$$\sum_{k''=1}^{N} (-1)^{|\sigma_k|} A_1^{\varrho_i\sigma_k} A_{M-1}^{\varrho_k\sigma_j} = \sum_{k=0}^{N} (-1)^{|\sigma_k|} A_1^{\varrho_k\sigma_j} A_{M-1}^{\varrho_i\sigma_k} \tag{29}$$

$$i = 1, 2, \ldots, N, \; j = 1, 2, \ldots, N$$

In such a way, some relationship is established among $A_M^{\rho_k\sigma_j}$ and $A_M^{\rho_i\sigma_k}$ polynomials, $k = 1, 2, \ldots, N$, and the idea will be elaborated in more detail in Section 6 which treats fasciagraphs with $l = 1$.

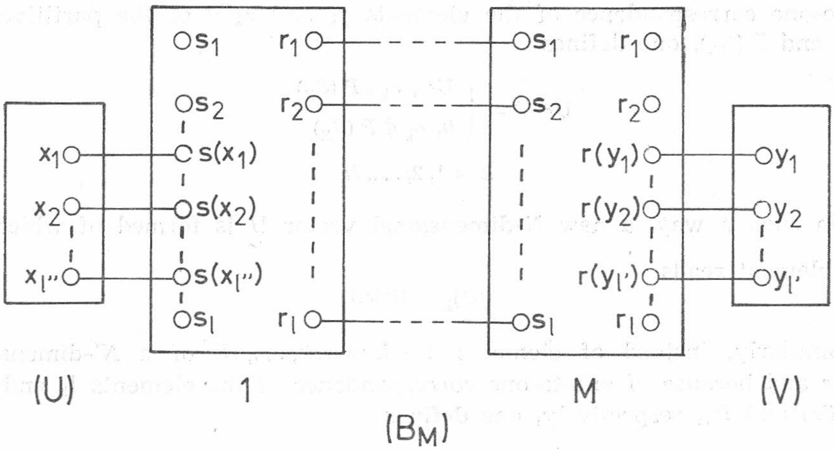
We would like to comment on the use of the recursive relations (26) and (27). We have adopted the following scheme: Polynomials $A_M^{\rho_i\sigma_j}$ are defined for $M > 0$ by their graphs while polynomials $A_0^{\rho_i\sigma_j}$ are given by eq. (15). Polynomials $A_1^{\rho_i\sigma_j}$, $A_2^{\rho_i\sigma_j}, \ldots, A_{N-1}^{\rho_i\sigma_j}$ can be easily evaluated explicitly by application of eq. (16). After that, higher order polynomials $A_M^{\rho_i\sigma_j}$, $M > N$, 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 $x_1 x_2, \ldots, x_{1''}$ form the set $X \subseteq U$. Its partitive set is $P(X)$ and the elements of $P(X)$ are denoted by χ_k, $k = 1, 2, \ldots, N''$. As before N'' stands for $2^{1''}$.



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 $\sigma_k^{(X)} \varepsilon P(S_X)$, $k = 1,2, \ldots, N''$.

Similarly, starting with $Y = \{y_1, y_2, \ldots, y_l\}$ 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 $|\varrho_k^{(Y)}| = |\mathrm{l}_k|$ where $\varrho_k^{(Y)} \varepsilon P(R_Y)$, $k = 1, 2, \ldots, N'$.

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

By applying the recurrsion 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:

$$B_M = \sum_{k'=1}^{N'} \sum_{k''=1}^{N''} (-1)^{|\varrho_{k'}^{(Y)}|} V^{\mathrm{l}_{k'}} (-1)^{|\sigma_{k''}^{(X)}|} A_M^{\varrho_{k'}^{(Y)} \sigma_{k''}^{(X)}} U^{\chi_{k''}} \tag{30}$$

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

$$A_M^{\varrho_{k'}^{(Y)} \sigma_{k''}^{(X)}}, \ M \geq N, \text{ one obtains}$$

$$\sum_{k=0}^{N} (-1)^k s_k B_{M-k} = 0, \ M \geq N, \tag{31}$$

namely, the acyclic polynomials B_M, $M \geq N$, obey the same recursive relation as do the polynomials $A_M^{\varrho_i \sigma_j}$. 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 $A_M^{\varrho_i \sigma_j}$, $M \geq N$, share the same inner fragment.

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

$$U^{\chi(\sigma_k)} = \begin{cases} U^{\chi_k}, & \sigma_k \varepsilon P(S_X) \\ 0, & \sigma_k \notin P(S_X) \end{cases} \tag{32a}$$

$$k = 1, 2, \ldots, N$$

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

$$(\underset{\sim}{U})_k = U^{\chi(\sigma_k)} \tag{32b}$$

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

$$V^{l(\varrho_k)} = \begin{cases} V^{l_k}, & \varrho_k \varepsilon P(P_Y) \\ 0, & \varrho_k \notin P(R_Y) \end{cases} \tag{33a}$$

$$k = 1, 2, \ldots, N$$

In such a way, a new N-dimensional vector $\underset{\sim}{W}$ is formed

$$(\underset{\sim}{W})_k = (-1)^{|\varrho_k|} V^{l(\rho_k)} \tag{33}$$

Eq. (30) is now rewritten as follows:

$$B_M = \sum_{k'=1}^{N} \sum_{k''=1}^{N} (W^t)_{k'} \cdot (-1)^{|\sigma k''|} A_M^{\sigma k' \sigma k''} (\underset{\sim}{U})_{k''} \tag{34}$$

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

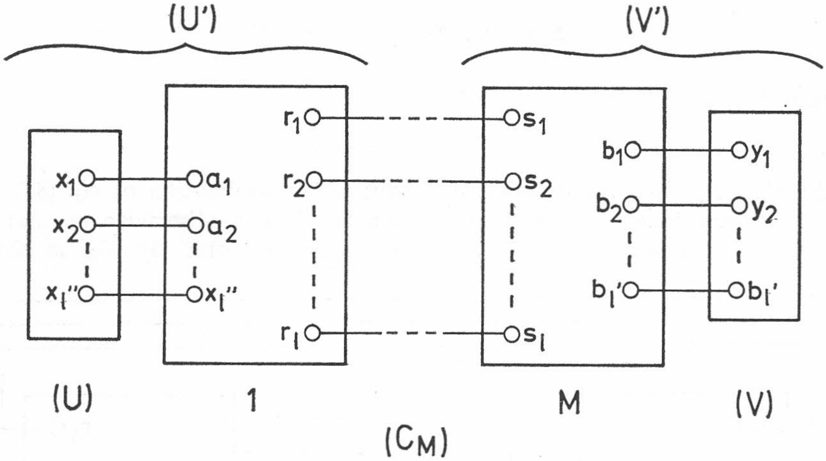
$$B_M = \underset{\sim}{W}^t T_M \underset{\sim}{U} = \underset{\sim}{W}^t T_1{}^M \underset{\sim}{U} \tag{35}$$

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

$$B_0 = \underset{\sim}{W}^t \underset{\sim}{U} \tag{36}$$

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 necessarilly 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 $A_M{}^{\rho_i\sigma_j}$ 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



$$C_M = W'^t\, T_1^{M-2}\, U' \tag{37}$$

where

$$(U')_k = U'^{\rho_k},\ (W')_k = (-1)^{|\sigma_k|} V'^{\sigma_k}, \tag{38}$$

where ϱ_k and σ_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:

$$\sum_{k=0}^{N} (-1)^k s_k C_{M-k} = 0,\ M \geq N + 2, \tag{39}$$

where the initial condition is given by

$$C_2 = W'^t \cdot U' \tag{40}$$

The same form of recurrence formulae (27), (31) and (39) is a topological consequence of all the polymers $A_M^{\rho_i\sigma_j}$, 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

$$U_M = \sum_{k=1}^{N} (-1)^{|\sigma_k|} A_M^{\rho_k\sigma_k} \tag{41}$$

Because of eqs. (16)—(17), one recognizes the diagonal terms of T_1^M and, therefore, one has

$$U_M = \mathrm{tr}\, T_M = \mathrm{tr}\, T_1^M. \tag{42}$$

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

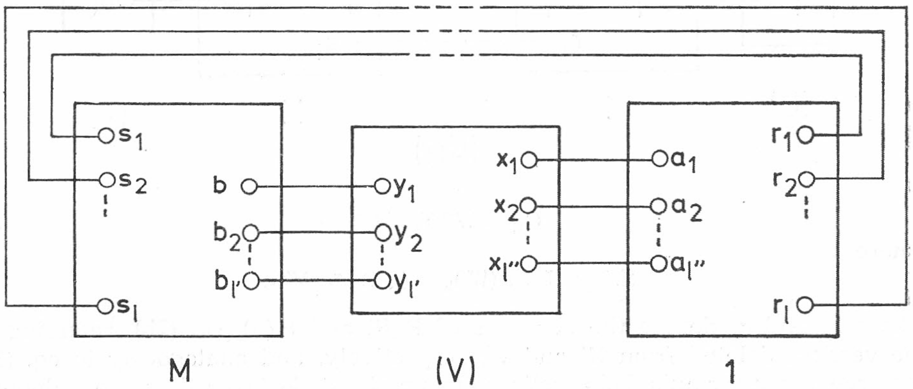
$$\sum_{k=0}^{N} (-1)^k s_k U_{M-k} = 0, \; M \geq N \tag{43}$$

The initial condition reads formally as

$$U_0 = \operatorname{tr} I = N \tag{44}$$

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 rotagraph. In such a way, the following derivative, denoted by V_M, is obtained



(V_M)

Treating the union of V and two neighbouring monomer units as one fragment V', one has for the acyclic polynomial of V_M

$$V_M = \sum_{i=1}^{N} \sum_{j=1}^{N} (-1)^{|\sigma_j|} A_{M-2}{}^{\rho_i \sigma_j} (-1)^{|\sigma_i|} V'^{\rho_j \sigma_i} \tag{45}$$

Let us introduce the matrix W' in the following way:

$$(W')_{ij} = (-1)^{|\sigma_j|} V'^{\rho_i \sigma_j} \tag{46}$$

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

$$V_M = \operatorname{tr} (T_1{}^{M-2} W') \tag{47}$$

and one gets the following recursion for polynomials V_M:

$$\sum_{k=0}^{N} (-1)^k s_k V_{M-k} = 0, \; M \geq N + 2 \tag{48}$$

with the initial condition given by

$$V_2 = \operatorname{tr} W' \tag{49}$$

Because all the systems considered, $A_M{}^{\varrho_i \sigma_j}$, 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 ROTAGRAPH

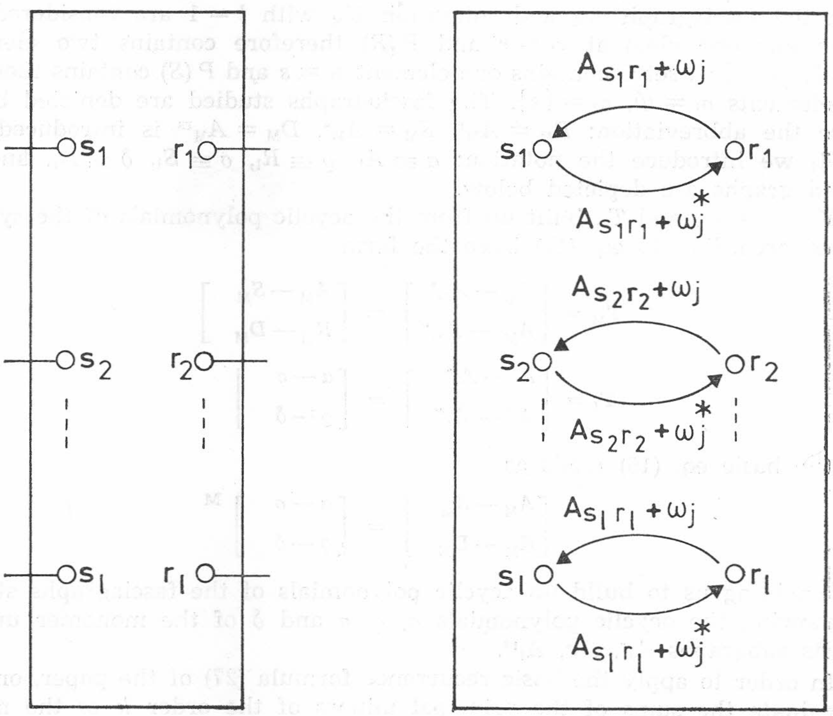
Heilbronner's recurrence formula for the characteristic polynomial $\overline{G}$ of a graph G as applied to an edge of G is given by eq. (3). Its repeated application to the edges of a fasciagraph A_M soon leads to involved expressions. The source of difficulties lies in the deletion of all cycles containing the edge under consideration. However, the formulae for the characteristic polynomial of a dimer as well as of regular conjugated polymers can be derived[14] 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 $\overline{A}_M$. The subject will be treated in the next section.

When the characteristic polynomial $\overline{U}_M$ 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 $\overline{U}_M$ factorizes as follows[1]:

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

where $\overline{A}(\omega_j)$ is the characteristic polynomial of the representative graph[15] $A(\omega_j)$ and $\omega_j = \exp(ij\,2\,\pi/M)$, $j = 1, 2, \ldots, M$, $i = \sqrt{-1}$, is related to the j th



(A(ωj))

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:

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

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

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

where ω_j^* denotes the complex conjugate of ω_j.

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

In fasciagraphs, 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 fasciagraph 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 $\varrho_1 = \Phi$, $\varrho_2 = \{r\}$; set S contains one element $s_1 = s$ and $P(S)$ contains therefore two elements $\sigma_1 = \Phi$, $\sigma_2 = \{s\}$. The fasciagraphs 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: $\alpha \equiv A_1$, $\varrho \equiv R_1$, $\sigma \equiv S_1$, $\delta \equiv D_1$, 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

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

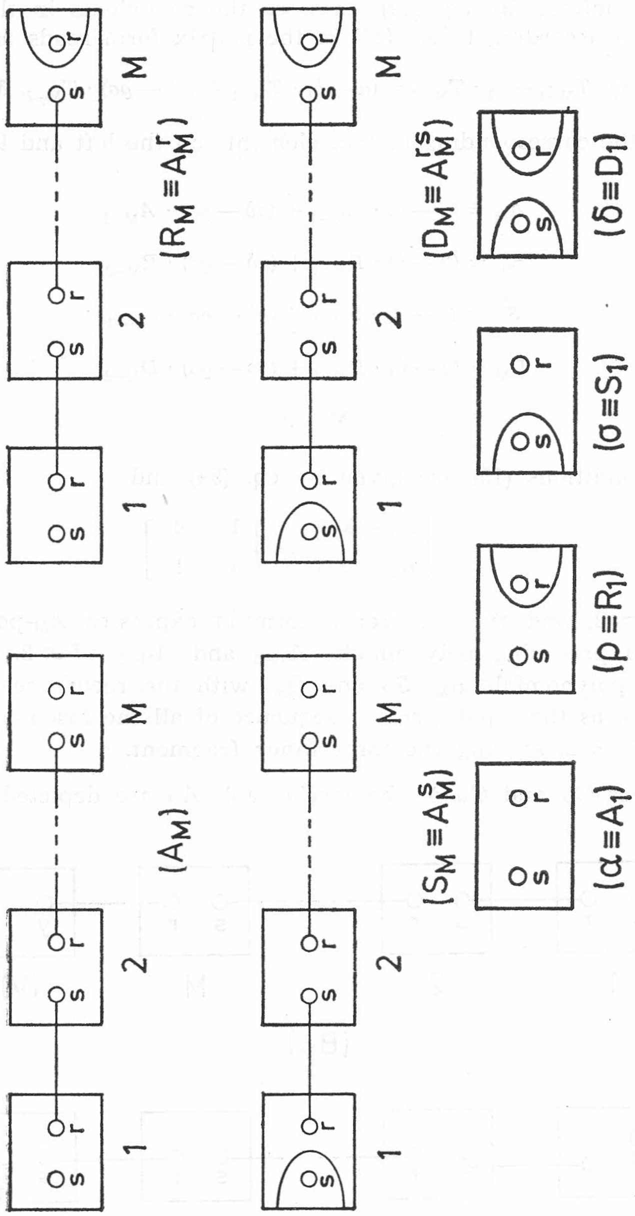
$$T_1 = \begin{bmatrix} A_1 - A_1{}^s \\ A_1{}^r - A_1{}^{rs} \end{bmatrix} = \begin{bmatrix} \alpha - \sigma \\ \varrho - \delta \end{bmatrix} \tag{54}$$

and the basic eq. (16) reads as

$$\begin{bmatrix} A_M - S_M \\ R_M - D_M \end{bmatrix} = \begin{bmatrix} \alpha - \sigma \\ \varrho - \delta \end{bmatrix}^M \tag{55}$$

thus enabling us to build up acyclic polynomials of the fasciagraphs studied by knowing the acyclic polynomials α, ϱ, σ and δ 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 $2^l = 2$)



(A_M)
(R_M ≡ A_M^r)
(S_M ≡ A_M^s)
(D_M ≡ A_M^rs)
(α ≡ A_1)
(ρ ≡ R_1)
(σ ≡ S_1)
(δ ≡ D_1)

$$s_0 = 1,\ s_2 = (\alpha - \delta),\ s_2 = \begin{vmatrix} \alpha - \sigma \\ \varrho - \delta \end{vmatrix} = -(\alpha\delta - \varrho\sigma) \tag{56}$$

Quantities s_k defined by eq. (19) serve as the coeficients in the recurrence formula which according to eq. (25) in the matrix form reads as

$$T_M = s_1 \cdot T_{M-1} - s_2 \cdot T_{M-2} = (\alpha - \delta) \cdot T_{M-1} + (\alpha\delta - \varrho\sigma) \cdot T_{M-2},\ M \geq 2; \tag{57}$$

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

$$A_M = (\alpha - \delta) \cdot A_{M-1} + (\alpha\delta - \varrho\sigma) \cdot A_{M-2} \tag{58a}$$

$$R_M = (\alpha - \delta) \cdot R_{M-1} + (\alpha\delta - \varrho\sigma) \cdot R_{M-2} \tag{58b}$$

$$S_M = (\alpha - \delta) \cdot S_{M-1} + (\alpha\delta - \varrho\sigma) \cdot S_{M-2} \tag{58c}$$

$$D_M = (\alpha - \delta) \cdot D_{M-1} + (\alpha\delta - \varrho\sigma) \cdot D_{M-2} \tag{58d}$$

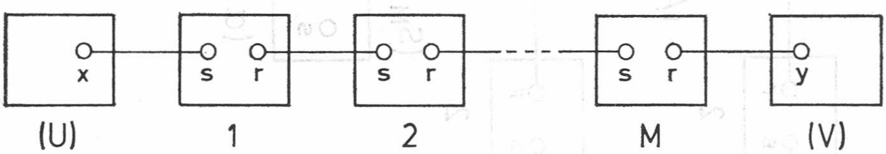
$$M \geq 2$$

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

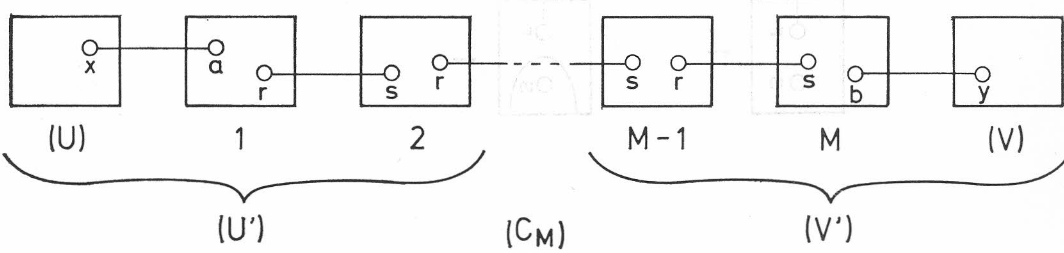
$$T_0 = \begin{bmatrix} A_0 - S_0 \\ R_0 - D_0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{59}$$

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 formulae of the same form as the topological consequence of all the fasciagraphs 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



(B_M)



(C_M)

and according to eqs. (35) and (37), one can express the acyclic polynomials of B_M and C_M as

$$B_M = [V - V^y] \begin{bmatrix} \alpha - \sigma \\ \varrho - \delta \end{bmatrix}^M \begin{bmatrix} U \\ U^x \end{bmatrix} \tag{60}$$

and

$$C_M = [V' - V^y] \begin{bmatrix} \alpha - \sigma \\ \varrho - \delta \end{bmatrix}^M \begin{bmatrix} U' \\ U'^x \end{bmatrix} =$$

$$= [V - V^y] \begin{bmatrix} A_1 - A_1^s \\ A_1^b - A^{bs} \end{bmatrix} \begin{bmatrix} \alpha - \sigma \\ \varrho - \delta \end{bmatrix}^{M-2} \begin{bmatrix} A_1 - A_1^a \\ A_1^r - A_1^{ra} \end{bmatrix} \begin{bmatrix} U \\ U^x \end{bmatrix} \tag{61}$$

Recurrence formulae have the form of eqs. (58)

$$B_M = (\alpha - \delta) \cdot B_{M-1} + (\alpha\delta - \varrho\sigma) \cdot B_{M-2} \tag{62}$$

$$M \geq 2$$

$$C_M = (\alpha - \delta) \cdot C_{M-1} + (\alpha\delta - \varrho\sigma) \cdot C_{M-2} \tag{63}$$

$$M \geq 4$$

with the initial conditions given by

$$B_0 = V \cdot U - V^y \cdot U^x \tag{64}$$

$$C_2 = V' \cdot U' - V'^y \cdot U'^x \tag{65}$$

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

$$A_{M+1} = \alpha \cdot A_M - \sigma \cdot R_M \tag{66}$$

$$A_{M+1} = \alpha \cdot A_M - \varrho \cdot S_M \tag{67}$$

and comparison of both formulae gives

$$R_M/S_M = \varrho/\sigma \text{ for all } M \tag{68}$$

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

$$R_{M+1} = \varrho \cdot A_M - \delta \cdot R_M \tag{69}$$

$$R_{M+1} = \alpha \cdot R_M - \varrho \cdot D_M \tag{70}$$

and comparison gives

$$\frac{A_M + D_M}{R_M} = \frac{\alpha + \delta}{\varrho} \text{ for all } M \tag{71}$$

In a completely analogous manner, one has

$$S_{M+1} = \alpha \cdot S_M - \sigma \cdot D_M \tag{72}$$

$$S_{M+1} = \sigma \cdot A_M - \delta \cdot S_M \tag{73}$$

and

$$D_{M+1} = \varrho \cdot S_M - \delta \cdot D_M \tag{74}$$

$$D_{M+1} = \sigma \cdot R_M - \delta \cdot D_M \tag{75}$$

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

$$\varrho\, A_M = R_{M+1} + \delta \cdot R_M \tag{76}$$

$$\sigma\, R_M = D_{M+1} + \delta \cdot D_M \tag{77}$$

and its immediate consequence

$$(\varrho\sigma)\, A_M = D_{M+2} + 2\,\delta\, D_{M+1} + \delta^2\, D_M \tag{78}$$

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

$$R_M = \varrho\, Q_M, \quad S_M = \sigma\, Q_M \tag{79}$$

and comparison with eq. (71) clarifies their meaning as

$$Q_M = \frac{R_M}{\varrho} = \frac{A_M + D_M}{\alpha + \delta} \tag{80}$$

with the initial conditions being

$$Q_0 = 0; \quad Q_1 = 1 \tag{81}$$

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

$$Q_M = (\alpha - \delta)\, Q_{M-1} + (\alpha\delta - \varrho\sigma)\, Q_{M-2} \tag{82}$$

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 α, ϱ, σ and δ 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 α and δ,

$$A_M = P_M(\alpha, \delta) \tag{83}$$

then one has the relationship

$$D_M = -P_M(-\delta, -\alpha). \tag{84}$$

Further, one should verify that A_M and D_M may be defined by MXM determinants of the form

$$A_M = \begin{vmatrix} \alpha & \xi & 0 & 0 \cdots \\ 1 & \alpha & \xi & 0 \cdots \\ \eta & 1 & \alpha & \xi \cdots \\ \eta^2 & \eta & 1 & \alpha \cdots \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{vmatrix} \tag{85}$$

$$D_M = \begin{vmatrix} -\delta & \xi & 0 & 0 \cdots \\ 1 & -\delta & \xi & 0 \cdots \\ -\zeta & 1 & -\delta & \xi \cdots \\ \zeta^2 & \zeta & 1 & -\delta \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{vmatrix} \tag{86}$$

where

$$\xi = \varrho\sigma, \quad \eta = \delta/\varrho\sigma, \quad \zeta = -\alpha/\varrho\sigma \tag{87}$$

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

$$Q_M(\alpha, \delta) = -Q_M(-\delta, -\alpha). \tag{88}$$

$Q_M(\alpha, \delta)$ is given by

$$Q_M = \begin{vmatrix} 1 & \xi & 0 & 0 & \cdots & 0 \\ \eta & \alpha & \xi & 0 & & \cdot \\ \eta^2 & 1 & \alpha & \xi & & \cdot \\ \eta^3 & \eta & 1 & \alpha & & \cdot \\ \cdot & & & & & \\ \cdot & & & & & \\ \cdot & & & & & \\ \eta^{M-1} & \eta^{M-2} & \eta^{M-3} & \eta^{M-4} & \cdots & \alpha \end{vmatrix} \tag{89}$$

$$R_M = \varrho\, Q_M, \quad S_M = \sigma\, Q_M \tag{90}$$

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

$$A_M = \sum_{\lambda=0}^{[M/2]} (-1)^\lambda \xi^\lambda \cdot f^{(M,\lambda)}(\alpha, \delta) \tag{91}$$

where $f^{(M,\lambda)}(\alpha, \delta)$ is a polynomial in α and δ of the degree $(M - 21)$

$$f^{(M,\lambda)}(\alpha, \delta) = \sum_{j=0}^{M-2\lambda} a_j(M, \lambda)\, \alpha^{M-2\lambda-j}\, \delta^j \tag{92}$$

Reccurence formula (58a) for the A_M's results in a recursion for the $f^{(M,\lambda)}$'s

$$f^{(M,\lambda)} = f^{(M-2,\lambda-1)} + (\alpha\delta)\, f^{(M-2,\lambda)} + (\alpha - \delta)\, f^{(M-1,\lambda)} \tag{93}$$

and consequently in a recursion for the $a_j^{(M,\lambda)}$-coefficients

$$\begin{aligned} a_j^{(M,\lambda)} &= a_j^{(M-2,\lambda-1)} + a_{j-1}^{(M-1,\lambda)} \\ &\quad - a_{j-1}^{(M-1,\lambda)} + a_j^{(M-1,\lambda)} \\ j &= 0, 1, \ldots \lambda;\ \lambda = 0, 1, \ldots [M/2] \end{aligned} \tag{94}$$

One has $f^{(M,o)}\,(\alpha, \delta) = \alpha^M$ (this corresponds to deleting all linking bonds without their incident vertices in A_M) and therefore

$$a_o^{(M,o)} = 1 \tag{95}$$

The above condition determines the coefficients as

$$a_j^{(M,\lambda)} = (-1)^j \binom{M-\lambda-j}{\lambda} \binom{\lambda+j-1}{\lambda-1} \qquad \lambda \geq 1 \tag{96}$$

and the A_M-polynomials of fasciagraph with $l = 1$ are explicitly given in terms of α, ϱ, σ and δ as follows

$$A_M = \alpha^M + \sum_{\lambda=1}^{[M/2]} (-1)^\lambda (\varrho\,\sigma)^\lambda \sum_{j=0}^{M-2\lambda} (-1) \binom{M-\lambda-j}{\lambda} \cdot \binom{\lambda+j-1}{\lambda-1} \alpha^{M-2\lambda-j}\, \delta^j \tag{97}$$

The polynomials A_M, namely their related coefficients $a_j^{(M,\lambda)}$, $j = 0, 1, \ldots, \lambda$; $\lambda = 0, 1, \ldots, [M/2]$, are listed in Appendix 2. for $M = 7, 8, \ldots, 20$.

Because of

$$\sum_{j=0}^{\lambda} |\, a_i^{(M,\lambda)} \,| = \sum_{j=0}^{\lambda} \binom{M-\lambda-j}{\lambda} \binom{\lambda+j-1}{\lambda-1} = \binom{M}{2\lambda} \tag{98}$$

there are altogether $\binom{M}{2\lambda}$ contributions containing $(\varrho\,\sigma)^\lambda$ 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

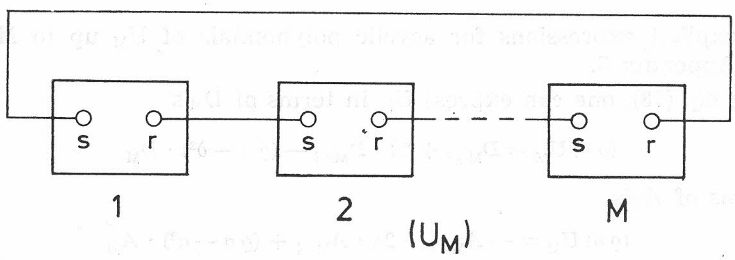
$$\sum_{\lambda=0}^{[M/2]_M} \binom{M}{2\,\lambda} = 2^{M-1} \tag{99}$$

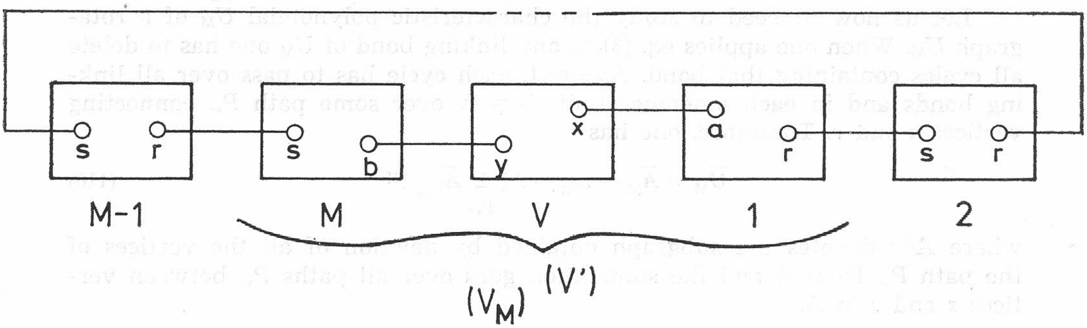
as the number of linking bonds in fasciagraph A_M is $(M - 1)$ and Heilbronner's-like formula (4) gives two contributions per each bond.

Let us now proceed to study the characteristic polynomials $\overline{A}_M$, $\overline{R}_M$, $\overline{S}_M$ and $\overline{D}_M$, $\overline{B}_M$ and $\overline{C}_M$ 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 formulae derived in the present chapter and the expressions listed in Appendix 1. and Appendix 2. are valid also for $\overline{A}_M$, $\overline{R}_M$, $\overline{S}_M$, $\overline{D}_M$, $\overline{B}_M$ and $\overline{C}_M$ after the appropriate change of acyclic polynomials (α, ϱ, σ, δ, etc.) by their corresponding characteristic polynomials ($\overline{\alpha}$, $\overline{\varrho}$, $\overline{\sigma}$, $\overline{\delta}$, etc.).

7. THE ACYCLIC AND THE CHARACTERISTIC POLYNOMIAL OF A ROTAGRAPH WITH l = 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

$$U_M = \mathrm{tr}\, T_M = \mathrm{tr} \begin{bmatrix} \alpha - \sigma \\ \varrho - \delta \end{bmatrix}^M \tag{100}$$

and

$$V_M = \mathrm{tr}\,(T_{M-2}\, W') = \mathrm{tr}\,(\begin{bmatrix} \alpha - \sigma \\ \varrho - \delta \end{bmatrix}^{M-2} \begin{bmatrix} V' & - V'^s \\ V'^r & - V'^{rs} \end{bmatrix}) \tag{101}$$

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

$$U_M = A_M - D_M \tag{102}$$

$$V_M = V' \cdot A_{M-2} - V'^r \cdot S_{M-2} - V'^s \cdot R_{M-2} + V'^{rs} \cdot D_{M-2} \tag{103}$$

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

$$U_M = (\alpha - \delta)\, U_{M-1} + (\alpha\, \delta - \varrho\, \sigma)\, U_{M-2} \tag{104}$$
$$M \geq 2$$

$$V_M = (\alpha - \delta)\, V_{M-1} + (\alpha\,\delta - \varrho\,\sigma)\, V_{M-2} \tag{105}$$
$$M \geq 4$$

with the initial conditions being

$$U_o = \operatorname{tr} I = 2 \tag{106}$$

$$V_2 = V' - V'^{rs} \tag{107}$$

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

$$(\varrho\,\sigma)\, U_M = D_{M+2} + 2\delta \cdot D_{M+1} - (\varrho\,\sigma - \delta^2) \cdot D_M \tag{108}$$

or in terms of A_M's

$$(\varrho\,\sigma)\, U_M = -A_{M+2} + 2\alpha \cdot A_{M+1} + (\varrho\,\sigma - \alpha^2) \cdot A_M \tag{109}$$

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

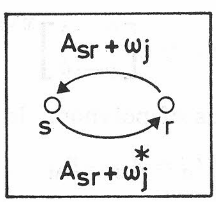
$$\overline{U}_M = \overline{A}_M - \overline{D}_M - 2\,[\sum_{P_{sr}} \overline{A}_{P_{sr}}\,]^M \tag{110}$$

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

$$\overline{U}_M = \overline{A}_M - \overline{D}_M - 2\,[\sum_{P_{sr}} \overline{A}^{P_{sr}}\,]^M = \prod_{j=1}^{M} \overline{A}\,(\omega_j) \tag{111}$$

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



$(A(\omega_j))$

The above equation clarifies the meaning of the important *topological function* $\overline{s}_2 = \overline{\alpha}\,\overline{\delta} - \overline{\varrho}\,\overline{\sigma}$ 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:

$$\overline{\alpha}\,\overline{\delta} - \overline{\varrho}\,\overline{\sigma} = -[\sum_{P_{sr}} \overline{A}^{P_{sr}}]^2 \tag{112}$$

namely, $\overline{s_2}$ 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[16] as a graph-theoretical reinterpretation of an older result[17].

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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 α, ϱ, σ and δ by $\overline{\alpha}$, $\overline{\varrho}$, $\overline{\sigma}$ and $\overline{\delta}$, respectively.

$Q_0 = 1$

$Q_1 = 1$

$$Q_2 = \frac{\alpha^2 - \delta^2}{\alpha + \delta}$$

$$Q_3 = \frac{\alpha^3 + \delta^3}{\alpha + \delta} - (\varrho\,\sigma)\,\frac{\alpha + \delta}{\alpha + \delta}$$

$$Q_4 = \frac{\alpha^4 - \delta^4}{\alpha + \delta} - (\varrho\,\sigma)\,2\,\frac{\alpha^2 - \delta^2}{\alpha + \delta}$$

$$Q_5 = \frac{\alpha^5 + \delta^5}{\alpha + \delta} - (\varrho\,\sigma)\,(3\,\frac{\alpha^3 + \delta^3}{\alpha + \delta} - \alpha\,\delta\,\frac{\alpha + \delta}{\alpha + \delta}) + (\varrho\,\sigma)^2$$

$$Q_6 = \frac{\alpha^6 - \delta^6}{\alpha + \delta} - (\varrho\,\sigma)\,(4\,\frac{\alpha^4 - \delta^4}{\alpha + \delta} - 2\,\alpha\,\delta\,\frac{\alpha^2 - \delta^2}{\alpha + \delta}) + (\varrho\,\sigma)^2\,3\,\frac{\alpha^2 - \delta^2}{\alpha + \delta}$$

$$A_0 = 1$$

$$A_1 = \alpha$$

$$A_2 = \alpha^2 - \varrho\,\sigma$$

$$A_3 = \alpha^3 - (\varrho\,\sigma)\,(2\alpha - \delta)$$

$$A_4 = \alpha^4 - (\varrho\,\sigma)\,(3\,\alpha^2 - 2\,\alpha\,\delta + \delta^2) + (\varrho\,\sigma)^2$$

$$A_5 = \alpha^5 - (\varrho\,\sigma)\,(4\,\alpha^3 - 3\,\alpha^2\,\delta + 2\,\alpha\,\delta^2 - \delta^3) + (\varrho\,\sigma)^2\,(3\,\alpha - 2\,\delta)$$

$$A_6 = \alpha^6 - (\varrho\,\sigma)\,(5\,\alpha^4 - 4\,\alpha^3\,\delta + 3\alpha^2\,\delta^2 - 2\,\alpha\,\delta^3 + \delta^4) + \\ + (\varrho\,\sigma)^2\,(6\,\alpha^2 - 6\,\alpha\,\delta + 3\,\delta^2) - (\varrho\,\sigma)^3$$

$$R_0 = 0$$

$$R_1 = \varrho$$

$$R_2 = \varrho\,(\alpha - \delta)$$

$$R_3 = \varrho\,[(\alpha^2 - \alpha\,\delta + \delta^2) - (\varrho\,\sigma)]$$

$$R_4 = \varrho\,[(\alpha^3 - \alpha^2\,\delta + \alpha\,\delta^2 - \delta^3) - (\varrho\,\sigma)\,(2\,\alpha - 2\,\delta)]$$

$$R_5 = \varrho[(\alpha^4 - \alpha^3\,\delta + \alpha^2 - \alpha\,\delta^3 + \delta^4) - (\varrho\,\sigma)(3\,\alpha^2 - 4\,\alpha\,\delta + 3\,\delta^2) + (\varrho\,\sigma)^2]$$

$$R_6 = \varrho\,[(\alpha^5 - \alpha^4\,\delta + \alpha^3\,\delta^2 - \alpha^2\,\delta^3 + \alpha\,\delta^4 - \delta^5) - (\varrho\,\sigma)\,(4\,\alpha^3 - 6\,\alpha^2\,\delta + 6\,\alpha\,\delta^2 - 4\,\delta^3) + \\ + (\varrho\,\sigma)^2\,(3\,\alpha - 3\,\delta)]$$

$$S_0 = 0$$

$$S_1 = \sigma$$

$$S_2 = \sigma\,(\alpha - \delta)$$

$$S_3 = \sigma\,[(\alpha^2 - \alpha\,\delta + \delta^2) - (\varrho\,\sigma)]$$

$$S_4 = \sigma\,[(\alpha^3 - \alpha^2\,\delta + \alpha\,\delta^2 - \delta^3) - (\varrho\,\sigma)\,(2\,\alpha - 2\,\delta)]$$

$$S_5 = \sigma\,[(\alpha^4 - \alpha^3\,\delta + \alpha^2\,\delta^2 - \alpha\,\delta^3 + \delta^3) - (\varrho\,\sigma)\,(3\,\alpha^2 - 4\,\alpha\,\delta + 3\,\delta^2) + (\varrho\,\sigma)^2]$$

$$S_6 = \sigma\,[(\alpha^5 - \alpha^4\,\delta + \alpha^3\,\delta^2 - \alpha^2\,\delta^3 + \alpha\,\delta^4 - \delta^5) - (\varrho\,\sigma)\,(4\,\alpha^3 - 6\,\alpha^2\,\delta + 6\,\alpha\,\delta^2 - 4\,\delta^3) + \\ + (\varrho\,\sigma)^2\,(3\,\alpha - 3\,\delta)]$$

$$D_0 = 1$$

$$D_1 = \delta$$

$$D_2 = -\delta^2 + (\varrho\,\sigma)$$

$$D_3 = \delta^3 - (\varrho\,\sigma)\,(2\,\delta - \alpha)$$

$$D_4 = -\delta^4 + (\varrho\,\sigma)\,(3\,\delta^2 - 2\,\alpha\,\delta + \alpha^2) - (\varrho\,\sigma)^2$$

$$D_5 = \delta^5 - (\varrho\,\sigma)\,(4\,\delta^3 - 3\,\delta^2\,\alpha + 2\,\delta\,\alpha^2 - \delta^3) + (\varrho\,\sigma)^2\,(3\,\delta - 2\,\alpha)$$

$$D_6 = -\delta^6 + (\varrho\,\sigma)\,(5\,\delta^4 - 4\,\delta^3\,\alpha + 3\,\delta^2\,\alpha^2 - 2\,\delta\,\alpha^3 + \alpha^4) - \\ - (\varrho\,\sigma)^2\,(6\,\delta^2 - 6\,\delta\,\alpha + 3\,\alpha^2) + (\varrho\,\sigma)^3$$

APPENDIX 2.

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

	$l = 0$	$l = 1$																		
M \ j	0	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			
18	120	—210	273	—312	330	—330	315	—288	252	—210	165	—120	78	—42	15		
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										
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	—200	150	—84	28								
13	120	—252	336	—350	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	1716	—2200	2475	—2520	2352	—2016	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	—1560	910	—420	120

$l = 4$

j / M	0	1	2	3	4	5	6	7	8	9	10	11	12
8	1												
9	5	—4											
10	15	—20	10										
11	35	—60	50	—20									
12	70	—140	150	—100	35								
13	126	—280	350	—300	175	—56							
14	210	—504	700	—700	525	—280	84						
15	330	—840	1260	—1400	1225	—840	420	—120					
16	495	—1320	2100	—2520	2450	—1960	1260	—600	165				
17	715	—1980	3300	—4200	4410	—3920	2940	—1800	825	—220			
18	1001	—2860	4950	—6600	7350	—7056	5880	—4200	2475	—1100	286		
19	1365	—4004	7150	—9900	11550	—11760	10584	—8400	5775	—3300	1430	—364	
20	1820	—5460	10010	—14300	17325	—18480	17640	—15120	11550	—7700	4290	—1820	455

$l = 5$

j / M	0	1	2	3	4	5	6	7	8	9	10
10	1										
11	6	—5									
12	21	—30	15								
13	56	—105	90	—35							
14	126	—280	315	—210	70						
15	252	—630	840	—735	420	—126					
17	792	—2310	1890	—1960	1470	—756	210				
16	462	—1260	3780	—4410	3920	—2646	1260	—330			
18	1287	—3960	6930	—8820	8820	—7056	4410	—1980	495		
19	2002	—6435	11880	—16170	17640	—15876	11760	—6930	2970	—175	
20	3003	—10010	19305	—27720	32340	—31752	26460	—18480	10395	—4290	—1001

$l = 6$

M \ j	0	1	2	3	4	5	6	7	8
12	1								
13	7	—6							
14	28	—42	21						
15	84	—168	147	—56					
16	210	—504	588	—392	126				
17	460	—1260	1764	—1568	882	—252			
18	942	—2772	4410	—4704	3528	—1764	462		
19	1716	—5544	9702	—11760	10584	—7056	3234	—792	
20	3003	—10296	19404	—25872	26460	—21168	12936	—5544	128

APPENDIX 3.

The explicit expressions in terms of α, ϱ, σ and δ polynomial for U_M acyclic polynomials up to $M = 6$ are given below.

$U_0 = 2$
$U_1 = \alpha - \delta$
$U_2 = (\alpha^2 + \delta^2) - 2\,(\varrho\,\sigma)$
$U_3 = (\alpha^3 - \delta^3) - 3\,(\varrho\,\sigma)\,(\alpha - \delta)$
$U_4 = (\alpha^4 + \delta^4) - 4\,(\varrho\,\sigma)\,(\alpha^2 - \alpha\,\delta + \delta^2) + 2\,(\varrho\,\sigma)^2$
$U_5 = (\alpha^5 - \delta^5) - 5\,(\varrho\,\sigma)\,(\alpha^3 - \alpha^2\,\delta + \alpha\,\delta^2 + \delta^3) + 5\,(\varrho\,\sigma)^2\;(\alpha - \delta)$
$U_6 = (\alpha^6 + \delta^6) - 6\,(\varrho\,\sigma)\,(\alpha^4 - \alpha^3\,\delta + \alpha^2\,\delta^2 - \alpha\,\delta^3 + \delta^4) + (\varrho\,\sigma)^2\,(9\,\alpha^2 - 12\,\alpha\,\delta +$
$+ 9\,\delta^2) - 2\,(\varrho\,\sigma)^3$

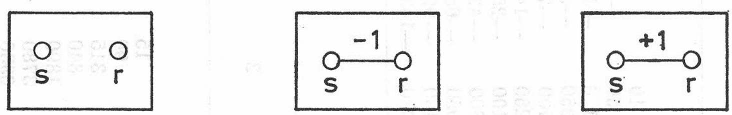
APPENDIX 4.

An Impirtant Topological Identity

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

$$\alpha^2 - 2\,\bar{\varrho}\,\bar{\sigma} + \bar{\delta}^2 - 2\,[\sum_{P_{sr}} \bar{A}^{P_{sr}}]^2 = \bar{A}\,(\omega_1 = -1) \cdot \bar{A}\,(\omega_2 = +1) \tag{4.1}$$

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



(A) (A(ω_1)) (A(ω_2))

Applying eq. (3) for $\bar{A}\,(\omega_1)$ and $\bar{A}\,(\omega_2)$ one has

$$\bar{A}\,(\omega_1) = \bar{\alpha} - \bar{\delta} + 2\,[\sum_{P_{sr}} \bar{A}_{P_{sr}}] \tag{4.2a}$$

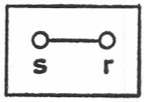
$$\bar{A}\,\omega_2) = \bar{\alpha} - \bar{\delta} - 2\,[\sum_{P_{sr}} \bar{A}^{P_{sr}}] \tag{4.2b}$$

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

$$\bar{\alpha} \cdot \bar{\delta} - \bar{\varrho} \cdot \bar{\sigma} = -\,[\sum_{P_{sr}} \bar{A}^{P_{sr}}]^2 \tag{4.3}$$

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

j \ M	$l = 7$							$l = 8$					$l = 9$			$l=10$
	0	1	2	3	4	5	6	0	1	2	3	4	0	1	2	0
14	1															
15	8	—7														
16	36	—56	28					1								
17	120	—252	224	—84				9	—8							
18	330	—840	1008	—672	210			45	—72	36			1			
19	792	—2310	3360	—3024	1680	—462		165	—360	324	—120		10	—9		
20	1716	—5544	9240	—10080	7560	—3696	924	495	—1320	1620	—1080	330	55	—90	45	1



(A')

It is obvious that

$$\overline{\varrho'} = \overline{\varrho}, \overline{\sigma'} = \overline{\sigma}, \overline{\delta'} = \overline{\delta} \tag{4.4}$$

and

$$\sum_{P_{sr}} \overline{A'}^{P_{sr}} = \overline{\delta} + \sum_{P_{sr}} \overline{A}^{P_{sr}} \tag{4.5}$$

as the edge connecting s and r is a path in A' but not in A.
Application of eq. (3) gives

$$\overline{\alpha'} = \overline{\alpha} - \overline{\delta} - 2\,[\sum_{P_{sr}} \overline{A}^{P_{sr}}] \tag{4.6}$$

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

$$\overline{\alpha'} \cdot \overline{\delta'} - \overline{\varrho'} \cdot \overline{\sigma'} = -\,[\sum_{P_{sr}} A'^{P_{sr}}]^2 \tag{4.7}$$

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

SAŽETAK

Aciklički i karakteristični polinom regularnih konjugiranih polimera i njihovih derivata

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

Za regularni polimer sa l veza među monomernim jedinicama prvo se konstruira $2^l \times 2^l$ polinomna 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^M, gdje M označava stupanj polimerizacije promatranog polimera. Aciklički polinom rotagrafa (koji predstavlja polimer zatvoren na samom sebi) jednak je tragu matrice T_1^M.

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

Za 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.