Journal of Mathematical Chemistry 8(1991)345–354

ON THE CHARACTERISTIC POLYNOMIALS OF SPIROGRAPHS AND RELATED GRAPHS

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Received 11 November 1990; revised 25 February 1991

Abstract

General recursive techniques are used to determine recurrence relations for the characteristic polynomials of graphs associated with various ring compounds.

1. Introduction

This note may be seen as a supplement to the recent paper [1] which reviews means of calculating the characteristic polynomial of a chemical graph. The purpose is to demonstrate the use of a recursive method for evaluating the characteristic polynomial $\phi_G(x)$ of an arbitrary multigraph G without recourse to either (a) the matching polynomial of G, or (b) the identification of all cycles or paths in G which contain a specified vertex or edge. The algorithm concerned is applied in section 3 to a type of cactus graph closely related to the spirographs considered in [2]. There, the author obtains recurrence relations for the characteristic polynomials of *linear* spirographs constructed from 3-cycles or 6-cycles: these are of the type illustrated in fig. 1, where $k \geq 3$, $1 \leq a \leq [k/2]$ and labels indicate the number of edges in a path. The relations obtained in [2] are improved in [3], where results for further values of k and a are obtained.

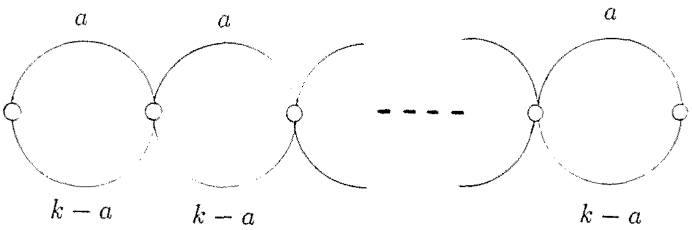

Fig. 1. A spirograph constructed from k-cycles.

Although it is asserted in [2] that "there are no general recursive procedures for all graphs", some such procedures are discussed in [1], while others have appeared in the mathematical literature. Among the first to be formulated was the following result of Schwenk [4, theorem 2]; others are given below and in [5, theorem 1], [6, theorem 2]. Here, $G - v$ denotes the graph obtained from G by deleting v and all edges containing v, notation which is extended in the natural way to deal with deleted sets of vertices.

PROPOSITION 1

Let v be a vertex of the graph G and let C be the collection of all cycles in G which contain v. Then,

$$\phi_G(x) = x\phi_{G-v}(x) - \sum_{u \sim v} \phi_{G-u-v}(x) - 2\sum_{Z \in C} \phi_{G-V(Z)}(x),$$

where $\sum_{u \sim v}$ denotes the sum over all vertices u adjacent to v. □

This result is proved using Sachs' interpretation of the coefficients of a characteristic polynomial in terms of a graph's cyclic structure (cf. [1, section 4] and [7, theorem 1.3]). As noted in [8], one consequence is the following result which justifies the "method of pruning spiral vertices" used in [2].

PROPOSITION 2

Let G be a graph obtained from disjoint graphs H, K by amalgamating vertex u of H with vertex v of K. Then,

$$\phi_G(x) = \phi_H(x)\phi_{K-v}(x) + \phi_{H-u}(x)\phi_K(x) - x\phi_{H-u}(x)\phi_{K-v}(x).$$

Proof

[4, corollary 2b]. An alternative derivation is given in [9, remark 1.6]. □

In section 2, we use proposition 2 to deal in general with the characteristic polynomials of spirographs of the type shown in fig. 1. The means of reducing hybrid recurrence relations to pure recurrence relations is essentially the "operator technique" of Hosoya and Ohkami [10]. They obtained their initial relations by repeated application of a reduction formula equivalent to the following result of Schwenk [4, theorem 3]; this is an analogue of proposition 1 for the graph $G - uv$ obtained from G by deleting the edge uv.

PROPOSITION 3

Let uv be an edge of the graph G, and let C be the collection of all cycles in G which contain uv. Then,

$$\phi_G(x) = \phi_{G-uv}(x) - \phi_{G-u-v}(x) - 2\sum_{Z \in C} \phi_{G-V(Z)}(x). \qquad \square$$

Hosoya and Ohkami found recurrence relations for the characteristic polynomials of certain polyhex graphs associated with benzene rings (cf. [11, section 5.13]), in particular a fourth-order relation for those of the type illustrated in fig. 2. The eigenvalues of these graphs (i.e. the roots of their characteristic polynomials) had been found some thirty-five years earlier by Coulson [12] and Rutherford [13]. Such graphs are formed from hexagons by amalgamating edges, whereas spirographs are formed from cycles by amalgamating vertices. An analogue of proposition 2 for the amalgamation of an edge is given in [14, proposition 2.4] as an application of the following algorithm [9, theorem 1.3].

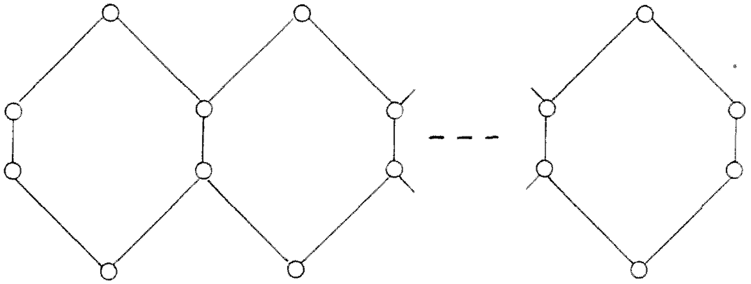

Fig. 2. A simple type of polyhex graph.

PROPOSITION 4 (The deletion–contraction algorithm)

Let G be a finite multigraph with at least three vertices, let u, v be distinct vertices of G, and let m be the number of edges between u and v. Let $G - [uv]$ be the multigraph obtained by deleting all m edges between u and v, and let G^* be the multigraph obtained from $G - [uv]$ by amalgamating u and v. Then,

$$\phi_G(x) = \phi_{G-[uv]}(x) + m\phi_{G^*}(x) + m(x-m)\phi_{G-u-v}(x) - m\phi_{G-u}(x) - m\phi_{G-v}(x). \quad \square$$

Unlike propositions 1 and 3, the deletion–contraction algorithm expresses $\phi_G(x)$ in terms of characteristic polynomials of *local* modifications of G (each with fewer edges than G when $m > 0$). Proposition 4 may be applied directly to the polyhex graph of fig. 2, but is seen to best advantage when the collection C of cycles specified in propositions 1 or 3 is unduly large. Such a situation arises in respect of the graph G_n^* obtained from the spirograph G_n of fig. 3 by amalgamating vertices u and v. Thus, G_n^* is a cyclic chain of triangles of interest in relation to spirocyclopropane compounds (where in practice n is even and $n \geq 10$). Note that in G_n^*, the vertices of degree 4 are no longer cutvertices and so proposition 2 is of no use in this context. In section 3, we use the deletion–contraction algorithm, together with the operator technique, to obtain a third-order recurrence relation for the characteristic polynomial of G_n^*.

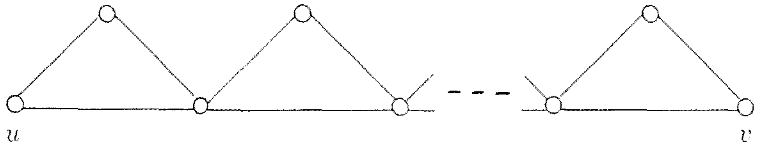

Fig. 3. A linear spirograph G_n constructed from n triangles.

Finally, we note that G_n^* has much greater symmetry than G_n; indeed, its automorphism group has only two orbits and this makes it possible to realize the characteristic polynomial of G_n^* as a product of quadratic factors, as described in [15]. This can, however, be achieved directly once we note that with an appropriate labelling of vertices, G_n^* has an adjacency matrix of the form

$$A = \begin{bmatrix} B & I+P \\ I+P^{-1} & 0 \end{bmatrix},$$

where B is the adjacency matrix of an n-cycle and P is a permutation matrix such that $P + P^{-1} = B$. Since $BP = PB$, we have $\det(xI - A) = \det\{xI(xI - B) - (I + P)(I + P^{-1})\} = \det\{(x^2 - 2)I - (x + 1)B\}$. In particular, -1 is not an eigenvalue of A and so all eigenvalues λ of G_n^* are obtained by setting $(\lambda^2 - 2)/(\lambda + 1)$ equal to an eigenvalue of B. The characteristic polynomial of G_n^* is now realized as $\prod_{j=1}^{n}\{x^2 - 2\alpha_j x - 2(1 + \alpha_j)\}$, where $\alpha_j = \cos(2\pi j/n)$.

2. Linear spirographs

For $n \geq 1$, let $X_n^{k,a}$ (or X_n when k and a are fixed) denote the graph constructed from n k-cycles, as illustrated in fig. 1, where $k \geq 3$ and $1 \leq a \leq [k/2]$. Let Y_n be the graph obtained from X_n by deleting the vertex shown in black in the figure; and let X_0 denote the trivial graph, Y_0 the empty graph. Additional notation is as follows: C_m ($m \geq 3$) denotes an m-cycle; P_m denotes an m-vertex path; the characteristic polynomial of the empty graph is to be interpreted as 1; and for clarity of exposition, a graph is identified with its characteristic polynomial.

We now apply proposition 2 to X_n, regarding X_n as the graph obtained by amalgamating a vertex of C_k with an appropriate vertex of X_{n-1}. We obtain

$$X_n = P_{k-1}X_{n-1} + C_kY_{n-1} - xP_{k-1}Y_{n-1}. \tag{2.1}$$

If we deal similarly with Y_n, then we obtain

$$Y_n = P_{a-1}P_{k-a-1}X_{n-1} + P_{k-1}Y_{n-1} - xP_{a-1}P_{k-a-1}Y_{n-1}. \tag{2.2}$$

Equations (2.1) and (2.2) may be written in the form:

$$\begin{bmatrix} X_n \\ Y_n \end{bmatrix} = M \begin{bmatrix} X_{n-1} \\ Y_{n-1} \end{bmatrix}, \text{ where } M = \begin{bmatrix} P_{k-1} & C_k - xP_{k-1} \\ P_{a-1}P_{k-a-1} & P_{k-1} - xP_{a-1}P_{k-a-1} \end{bmatrix}. \tag{2.3}$$

Now M satisfies its characteristic polynomial, that is,

$$M^2 - (2P_{k-1} - xP_{a-1}P_{k-a-1})M + (P_{k-1}^2 - C_kP_{a-1}P_{k-a-1})I = 0, \tag{2.4}$$

and so eq. (2.3) yields a second-order recurrence relation satisfied by both X_n and Y_n. In particular, we deduce the following result from eq. (2.4).

PROPOSITION 5

For the graph X_n of fig. 1, we have

$$X_n = (2P_{k-1} - xP_{a-1}P_{k-a-1})X_{n-1} + (C_kP_{a-1}P_{k-a-1} - P_{k-1}^2)X_{n-2} \quad (n \geq 2),$$

where $X_0 = x$ and $X_1 = C_k$. □

Characteristic polynomials of paths and cycles have simple expressions in terms of Chebyshev polynomials [7, p. 73] and these can make for some minor simplifications which we do not pursue here. The resulting recurrence relations for all $X_n^{k,a}$ with $3 \leq k \leq 6$ are given in [3, table 1]. Here, we note the results in just three cases: one is required in section 3, the second was derived incorrectly in [2], and the third is stated wrongly in [3].

PROPOSITION 6

(i) $X_n^{3,1} = (x^2 - 2)X_{n-1}^{3,1} - (x+1)^2X_{n-2}^{3,1} \quad (n \geq 2)$,

where $X_0^{3,1} = x$ and $X_1^{3,1} = x^3 - 3x - 2$.

(ii) $X_n^{4,2} = (x^3-4x)X_{n-1}^{4,2} - 4x^2X_{n-2}^{4,2} \quad (n \geq 2),$

where $X_0^{4,2} = x$ and $X_1^{4,2} = x^4 - 4x^2$.

(iii) $X_n^{6,3} = (x^5-6x^3+5x)X_{n-1}^{6,3} - (4x^4-8x^2+4)X_{n-2}^{6,3} \quad (n \geq 2),$

where $X_0^{6,3} = x$ and $X_1^{6,3} = x^6 - 6x^4 + 9x^2 - 4$. □

We note that for the graph $X_n^{4,2}$, the intermediate working in [2] is incorrect: eq. (4) there should read $h' = \lambda^3 - 2\lambda$ and eq. (7) should read $\det(A) = (\lambda^3 - 2\lambda)h - 2\lambda^2 h'$, with consequent amendments to eqs. (9), (10) and (13). Notwithstanding these errors, the characteristic polynomials obtained are correct, as can be seen by interpreting (h_n, h_n') in [2] as $(X_n, \frac{1}{2}x^{-1}X_n + \frac{1}{2}Y_n)$ instead of (X_n, Y_n) in the case $(k, a) = (4, 2)$.

3. Some more recurrence relations

In this section, we show how the deletion–contraction algorithm may be used to obtain directly a recurrence relation for the characteristic polynomials of the graphs G_n^* defined in section 1. The subgraphs of G_n^* which arise, together with an associated multigraph D_n, are illustrated in fig. 4 (where only a segment of each graph is shown). Here, $n \geq 2$, and G_2^* is a multigraph with a double edge.

On applying proposition 4 to G_n^*, D_n and L_n, with u, v the vertices shown in black, we obtain (for $n \geq 3$):

$$G_n^* = H_n + D_n + (x-1)E_n - L_n - Q_n, \tag{3.1}$$

$$D_n = G_{n-1} + 2G_{n-1}^* + 2(x-2)Q_{n-1} - 4E_n, \tag{3.2}$$

$$L_n = G_{n-1} + G_{n-1}^* + (x-1)Q_{n-1} - 2E_n. \tag{3.3}$$

Each of the graphs H_n, E_n, Q_n has a pendant vertex (shown in black) and accordingly we may invoke the following result: if the graph G' is obtained from a graph G by adding a pendant edge at vertex v, then

$$\phi_{G'}(x) = x\phi_G(x) - \phi_{G-v}(x). \tag{3.4}$$

This is a special case of proposition 2, but it also has a straightforward direct proof. On applying eq. (3.4) to H_n, E_n, Q_n, we obtain (for $n \geq 3$):

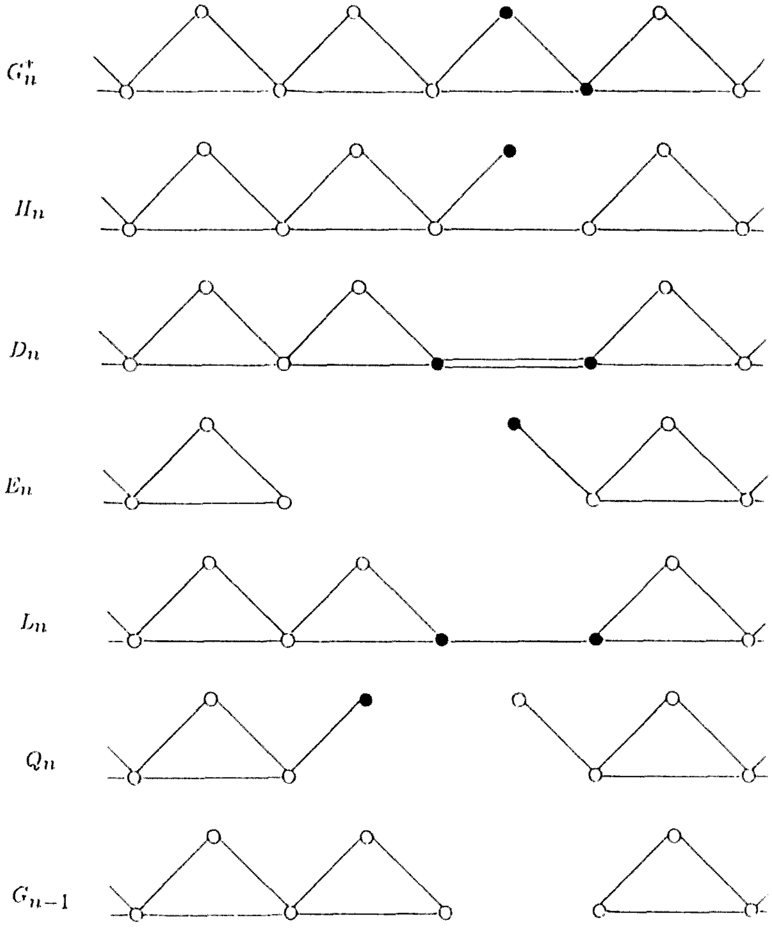

Fig. 4. Segments of G_n^* and associated graphs.

$$H_n = xL_n - E_n, \tag{3.5}$$

$$E_n = xG_{n-2} - E_{n-1}, \tag{3.6}$$

$$Q_n = xE_n - Q_{n-1}. \tag{3.7}$$

Finally, since G_n is the graph $X_n^{3,1}$ of proposition 6(i), we have (for $n \geq 3$):

$$G_n = (x^2 - 2)G_{n-1} - (x+1)^2 G_{n-2}. \tag{3.8}$$

We now have seven independent equations ((3.1) to (3.3) and (3.5) to (3.8)) relating the characteristic polynomials of the seven multigraphs derived from G_n^*. Accordingly, we may now apply the operator technique of [10]: we find that the shift operator **O** satisfies

Table 1

Coefficients in the characteristic polynomial G_n^* ($n = 1, \ldots, 8$)

n	a_{16}	a_{15}	a_{14}	a_{13}	a_{12}	a_{11}	a_{10}	a_9	a_8	a_7	a_6	a_5	a_4	a_3	a_2	a_1	a_0
1															1	–2	–4
2													1		–8	–8	
3											1		–9	–8	9	6	–4
4									1		–12	–8	36	32	–32	–32	
5							1		–15	–10	70	78	–100	–160	–15	30	–4
6					1		–18	–12	111	132	–242	–420	57	304	24	–72	
7			1		–21	–14	161	196	–497	–884	413	1358	175	–728	–231	70	–4
8	1		–24	–16	220	272	–888	–1616	1284	3904	304	–3680	–1648	896	384	–128	

$$(\mathbf{O} + 1)^2\{\mathbf{O} - (x + 1)\}\{\mathbf{O}^2 - (x^2 - 2)\mathbf{O} + (x + 1)^2\} = 0.$$

In particular, since $\mathbf{O}G_n^* = G_{n+1}^*$, we have for $n \geq 7$:

$$G_n^* = (x^2 + x - 3)G_{n-1}^* - (x^3 - 2x + 2)G_{n-2}^* - (x^3 - 4x - 2)G_{n-3}^* + (x + 1)(x^2 + 3x + 3)G_{n-4}^* + (x + 1)^3 G_{n-5}^*. \tag{3.9}$$

We define G_1^* as $x^2 - 2x - 4$, so that (3.9) holds for all $n \geq 6$. For subsequent reference, the coefficients in the characteristic polynomials $\sum_k a_k x^k$ of G_n^* ($n = 1$ to 8) are listed in table 1. (The data for the cases $n = 2, 3, 4, 5, 6$ represent the initial conditions for (3.9) and are found directly.)

We can now go on to show that G_n^* satisfies the third-order recurrence relation equivalent to the equation

$$\{\mathbf{O} - (x + 1)\}\{\mathbf{O}^2 - (x^2 - 2)\mathbf{O} + (x + 1)^2\}G_n^* = 0. \tag{3.10}$$

Equation (3.10) was derived in [3, section 3.1] by a method which requires both (a) the matching polynomial, and (b) identification of all cycles containing a specified edge.

PROPOSITION 7

We have

$$G_n^* = (x^2 + x - 1)G_{n-1}^* - (x^3 + 2x^2 - 1)G_{n-2}^* + (x + 1)^3 G_{n-3}^* \quad (n \geq 4),$$

where

$$G_1^* = x^2 - 2x - 4,\ G_2^* = x^4 - 8x^2 - 8x$$

and

$$G_3^* = x^6 - 9x^4 - 8x^3 + 9x^2 + 6x - 4.$$

Proof

From table 1, this third-order relation holds for $n = 4, 5, 6, 7, 8$. For $n \geq 9$, the result follows from (3.9) by induction on n. ☐

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