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CHARACTERISTIC POLYNOMIALS OF SPIROGRAPHS

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Abstract

A class of graphs called spirographs is defined. It is shown that the characteristic polynomials of spirographs can be obtained in terms of the characteristic polynomials of smaller graphs by pruning the spirographs at the spiral points. Elegant recursive relations are derived for many spirographs. Characteristic polynomials of branched spirographs are also obtained.

1. Introduction

The evaluation of the characteristic polynomials of graphs has been the subject of many investigations [1 – 40] in recent years. The evaluation of these polynomials for graphs is generally regarded as a tedious problem as a result of the combinatorial complexity. There are a number of chemical applications of these polynomials. Many of these applications are discussed in the references quoted above [1 – 34], but in particular in the recent references [10 – 13].

The characteristic polynomials of graphs have applications in chemical kinetics [37], dynamics of oscillatory reactions, quantum chemistry, determination of the stabilities of reaction networks [35], lattice statistics [38], estimation of the stabilities of conjugated systems [27], formulation of the TEMO theorem [39], enumeration of walks and self-returning walks [3], and electronic structure of organic polymers and periodic structures [4,11].

The present author [8,38] has been interested in deriving recursive methods to generate the characteristic polynomials of graphs. While there are no general recursive procedures for all graphs, recursive relations could be derived for some classes of graphs. The present author [8] developed an elegant tree-pruning procedure for the

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characteristic polynomials of graphs with pending bonds [9] and the characteristic polynomials of weighted trees and weighted structures with pending bonds [10]. More recently, the present author [38] showed that the method of tree pruning could be applied to the lattice statistics of Bethe lattices, which are used extensively in statistical mechanics.

In this investigation, we introduce a class of graphs called spirographs which are obtained by soldering cyclic graphs at single points. The spirographs introduced here appear in several chemical applications. Many silicates can be represented by spiral networks. Thus, the polynomials would be of use in classifying the networks. A class of spirographs called Cacti graphs are useful in lattice statistics in statistical mechanics. We develop recursive procedures for computing the characteristic polynomials of spirographs. The procedure is applied to a number of spirographs containing triangles, squares and hexagons. Section 2 describes the method of investigation. Section 3 comprises results and discussions.

2. Spirographs and their characteristic polynomials

A. SPIROGRAPHS

We coin the term 'spirographs' motivated by the term 'spirocycle' used in organic chemistry for a class of ring compounds which are obtained by joining two rings at a single vertex such that the two rings have only one common vertex. Figure 1 shows an example of a spirograph containing two '4-membered rings' or containing two 4-cycles.

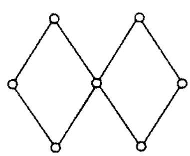


Fig. 1. A spirograph containing two squares.

A spirograph can be obtained from simple ring graphs by 'soldering' or joining a single vertex of one ring to a single vertex of another ring so that the two vertices are fused to become a single vertex in the final soldered graph. The resulting single vertex is called a spiral vertex in this investigation. We show here that the characteristic polynomials of spirographs can be obtained by pruning the spirograph at the spiral points. The general method of pruning was developed earlier for trees. We show here that when the pruning method is applied to spirographs correctly, one could generate the characteristic polynomials of spirographs. In section 2B, we briefly outline the pruning method.

B. PRUNING METHOD AND CHARACTERISTIC POLYNOMIALS

If the spirograph in fig. 1 is cut at the spiral point, one obtains the two graphs shown in fig. 2, with the spiral vertex identified by a closed circle. For convenience, let us call the first graph Q (the quotient graph) and the second graph T (the type). The graph in fig. 1 is then obtainable by joining the two black vertices (spiral vertices)

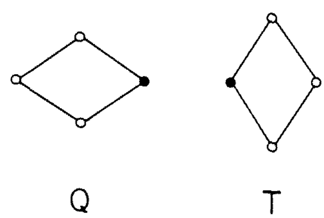


Fig. 2. The two graphs resulting from pruning the spirograph in fig. 1. The spiral vertex is the shaded vertex.

together into a single vertex. This procedure was formulated earlier for trees by the present author [41] and was called a root-to-root product. We show here that the characteristic polynomial of the original spirograph in fig. 1 can be obtained from the characteristic polynomials of the pruned graphs Q and T in fig. 2.

The characteristic polynomial of a graph G in general is defined as the secular determinant of the adjacency matrix A of the graph shown below:

$$P_G(\lambda) = |A - \lambda I|, \tag{1}$$

where the adjacency matrix A is defined as

$$A_{ij} = \begin{cases} 1 \text{ if } i \neq j \text{ and the} \\ \text{vertices } i \text{ and } j \text{ are connected} \\ \\ 0 \text{ otherwise.} \end{cases} \tag{2}$$

Let us consider the graphs in figs. 1 and 2 as examples. Let the characteristic polynomial of type T in fig. 2 be denoted by h. It can easily be verified that

$$h = \lambda^4 - 4\lambda^2. \tag{3}$$

Let T' be the graph obtained by deleting the spiral point (black vertex) of graph T in fig. 2. Let h' denote the characteristic polynomial of T with the spiral point deleted. It can easily be seen that h' is given by

$$h' = \lambda^3 - 3\lambda . \tag{4}$$

Define the reduced adjacency matrix of the quotient graph Q as follows:

$$A_{ij} = \begin{cases} -1 & \text{if } i \neq j,\ i \text{ and } j \text{ are connected, and } i \text{ is not a spiral vertex} \\ -h' & \text{if } i \neq j,\ i \text{ and } j \text{ are connected, and } i \text{ is a spiral vertex} \\ \lambda & \text{if } i = j \text{ and } i \text{ is not a spiral vertex} \\ h & \text{if } i = j \text{ and } i \text{ is a spiral vertex.} \end{cases} \tag{5}$$

The determinant of the matrix A is simply the characteristic polynomial of the original spirograph. For the example we started with, we show below the reduced adjacency matrix with the convention that vertex 1 is the spiral vertex:

$$A = \begin{bmatrix} h & -h' & 0 & -h' \\ -1 & \lambda & -1 & 0 \\ 0 & -1 & \lambda & -1 \\ -1 & 0 & -1 & \lambda \end{bmatrix} \tag{6}$$

The determinant of the above matrix is easily seen to be

$$\mathrm{Det}(A) = \lambda^3 h - 4\lambda^2 h' . \tag{7}$$

By substituting for h and h' the expressions (3) and (4) previously obtained, we find the characteristic polynomial of the original spirograph to be

$$\lambda^7 - 8\lambda^5 + 12\lambda^3 . \tag{8}$$

Consequently, in this case, the original problem of evaluating the characteristic polynomial of a graph which contains seven vertices is reduced into a problem of obtaining the characteristic polynomial of a simpler non-spiro graph containing four vertices. The procedure can be extended further to graphs which contain many spiral points. The resulting simplification grows exponentially (!) as the number of spiral points increases.

To illustrate the above point, consider the spirograph in fig. 3 which contains two spiral points. Let the characteristic polynomial of a spirograph containing n square rings be h_n. One can derive actually a recursive relation for h_n which can be solved iteratively. In the present example, we seek a solution for h_3. If one prunes the spirograph in fig. 3 at the first spiral vertex and applies the method outlined earlier, it can be shown that

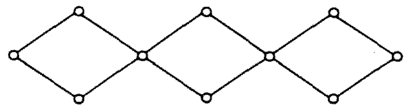


Fig. 3. A spirograph containing three squares.

$$h_3 = \lambda^3 h_2 - 4\lambda^2 h'_2 . \tag{9}$$

To obtain h_2, we prune the spirograph containing two squares. Thus, h_2 is given by

$$h_2 = \lambda^3 h_1 - 4\lambda^2 h'_1 . \tag{10}$$

The polynomial h'_2 is given by

$$h'_2 = \lambda^2 h_1 - 2\lambda h'_1 . \tag{11}$$

Thus, h_2 and h'_2 are determined if one can find h_1 and h'_1. The polynomials h_1 and h'_1 are simply the characteristic polynomials of a single 4-membered cycle and a chain containing three vertices, respectively. They are given by expressions (3) and (4), respectively. One can obtain h_2 and h'_2 from h_1 and h'_1; the polynomial h_3 can be obtained once h_2 and h'_2 are found. Thus, the final polynomial for the spirograph in fig. 3 is given by

$$h_3 = \lambda^{10} - 12\lambda^8 + 40\lambda^6 - 32\lambda^4 . \tag{12}$$

In this example, the characteristic polynomial of a spirograph containing ten vertices could be generated from the characteristic polynomial of a square graph and a chain containing three vertices.

The above procedure could be generalized to any spirograph containing n rings, For a linear spirograph which contains n square rings, we obtain the following recursive relations. Let h_n denote the polynomial of such a spirograph containing n rings. Using the pruning method developed earlier, the following relations can be derived:

$$\begin{aligned} h_n &= \lambda^2 h_{n-1} - 4\lambda^2 h'_{n-1} \\ h_{n-1} &= \lambda^2 h_{n-2} - 4\lambda^2 h'_{n-2} \\ &\;\vdots \\ h_2 &= \lambda^2 h_1 - 4\lambda h'_1 \\ h_1 &= \lambda^4 - 4\lambda^2 \\ h'_1 &= \lambda^3 - 3\lambda . \end{aligned} \tag{13}$$

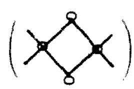
Thus, closed analytical solutions exist for the characteristic polynomials of linear-spirographs containing n square rings. As we show in the next section, similar recursive relationships can be obtained for many spirographs.

3. Results and discussion

In this section, we consider many classes of spirographs and derive recursive relationships and the actual characteristic polynomials.

For the linear-square-spirographs, the recursive relations (13) for the characteristic polynomials were derived in section 2B. Table 1 shows the actual characteristic

Table 1

Characteristic polynomials of linear-square-spirographs  $_n$

n	Polynomial
1	$\lambda^4 - 4\lambda^2$
2	$\lambda^7 - 8\lambda^5 + 12\lambda^3$
3	$\lambda^{10} - 12\lambda^8 + 40\lambda^6 - 32\lambda^4$
4	$\lambda^{13} - 16\lambda^{11} + 84\lambda^9 - 160\lambda^7 + 80\lambda^5$
5	$\lambda^{16} - 20\lambda^{14} + 144\lambda^{12} - 448\lambda^{10} + 560\lambda^8 - 192\lambda^6$
6	$\lambda^{19} - 24\lambda^{17} + 220\lambda^{15} - 960\lambda^{13} + 2016\lambda^{11} - 1792\lambda^9 + 448\lambda^7$
7	$\lambda^{22} - 28\lambda^{20} + 312\lambda^{18} - 1760\lambda^{16} + 5280\lambda^{14} - 8064\lambda^{12} + 5376\lambda^{10} - 1024\lambda^8$
8	$\lambda^{25} - 32\lambda^{23} + 420\lambda^{21} - 2912\lambda^{19} + 11\,440\lambda^{17} - 25\,344\lambda^{15} + 29\,568\lambda^{13} - 15\,360\lambda^{11} + 2304\lambda^9$
9	$\lambda^{28} - 36\lambda^{26} + 544\lambda^{24} - 4480\lambda^{22} + 21\,840\lambda^{20} - 64\,064\lambda^{18} + 109\,824\lambda^{16} - 101\,376\lambda^{14} + 42\,240\lambda^{12} - 5120\lambda^{10}$
10	$\lambda^{31} - 40\lambda^{29} + 684\lambda^{27} - 6528\lambda^{25} + 38\,080\lambda^{23} - 139\,776\lambda^{21} + 320\,320\lambda^{19} - 439\,296\lambda^{17} + 329\,472\lambda^{15} - 112\,640\lambda^{13} + 11\,264\lambda^{11}$

polynomials for linear-square-spirographs for n = 1 to 10. All the polynomials shown in the table were obtained using the recursive relation derived in section 2B from simply the characteristic polynomial of a cycle containing four vertices (C_4) and a linear chain containing three vertices (l_3).

Next, we consider a set of linear-triangle-spirographs. Figure 4 shows an example of a linear-triangle-spirograph containing six rings. The method of pruning the spirograph at the spiral points can be applied to the triangle spirographs. Let h_n denote the characteristic polynomial of a triangle spirograph which contains n rings. The the recursive relations for h_n's are shown in table 2. Table 3 shows the actual characteristic polynomials of linear spirographs containing ten or less triangles.

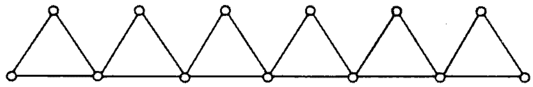
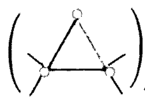


Fig. 4. A linear spirograph which contains six triangles.

Table 2

Recursive relations for the linear-triangle spirographs  $_n$

h_1		$\lambda^3 - 3\lambda - 2$
h'_1		$\lambda^2 - 1$
h_2		$\lambda h_1^2 - \lambda h_1'^2 - 2h_1 h'_1 - 2h_1'^2$
h'_2		$\lambda h_1 - h'_1$
		. . .
h_n	=	$\lambda h_{n-1}^2 - \lambda h_{n-1}'^2 - 2h_{n-1} h'_{n-1} - 2h_{n-1}'^2$

Table 3

Characteristic polynomials of spiro-triangle-graphs (n = 1, 10)

n	Polynomial
1	$\lambda^3 - 3\lambda - 2$
2	$\lambda^5 - 6\lambda^3 - 4\lambda^2 + 5\lambda + 4$
3	$\lambda^7 - 9\lambda^5 - 6\lambda^4 + 19\lambda^3 + 20\lambda^2 - 3\lambda - 6$
4	$\lambda^9 - 12\lambda^7 - 8\lambda^6 + 42\lambda^5 + 48\lambda^4 - 32\lambda^3 - 56\lambda^2 - 7\lambda + 8$
5	$\lambda^{11} - 15\lambda^9 - 10\lambda^8 + 74\lambda^7 + 88\lambda^6 - 114\lambda^5 - 204\lambda^4 + \lambda^3 + 112\lambda^2 + 29\lambda - 10$
6	$\lambda^{13} - 18\lambda^{11} - 12\lambda^{10} + 115\lambda^9 + 140\lambda^8 - 276\lambda^7 - 504\lambda^6 + 123\lambda^5 + 592\lambda^4 + 178\lambda^3 - 172\lambda^2 - 67\lambda + 12$
7	$\lambda^{15} - 21\lambda^{13} - 14\lambda^{12} + 165\lambda^{11} + 204\lambda^{10} - 545\lambda^9 - 1010\lambda^8 + 539\lambda^7 + 1944\lambda^6 + 453\lambda^5 - 1266\lambda^4 - 677\lambda^3 + 196\lambda^2 + 125\lambda - 14$
8	$\lambda^{17} - 24\lambda^{15} - 16\lambda^{14} + 224\lambda^{13} + 280\lambda^{12} - 948\lambda^{11} - 1776\lambda^{10} + 1510\lambda^9 + 4880\lambda^8 + 536\lambda^7 - 5488\lambda^6 - 3068\lambda^5 + 1952\lambda^4 + 1712\lambda^3 - 112\lambda^2 - 207\lambda + 16$
9	$\lambda^{19} - 27\lambda^{17} - 18\lambda^{16} + 292\lambda^{15} + 368\lambda^{14} - 1512\lambda^{13} - 2856\lambda^{12} + 3378\lambda^{11} + 10\,328\lambda^{10} - 458\lambda^9 - 17\,260\lambda^8 - 9020\lambda^7 + 11\,344\lambda^6 + 10\,604\lambda^5 - 1592\lambda^4 - 3471\lambda^3 - 192\lambda^2 + 317\lambda - 18$
10	$\lambda^{21} - 30\lambda^{19} - 20\lambda^{18} + 369\lambda^{17} + 468\lambda^{16} - 2264\lambda^{15} - 4304\lambda^{14} + 6566\lambda^{13} + 19\,432\lambda^{12} - 4224\lambda^{11} - 44\,040\lambda^{10} - 19\,910\lambda^9 + 45\,400\lambda^8 + 42\,152\lambda^7 - 14\,608\lambda^6 - 27\,227\lambda^5 - 2272\lambda^4 + 5978\lambda^3 + 876\lambda^2 - 459\lambda + 20$

In comparing the results in tables 1 and 3, we note that the coefficient of the second term in the characteristic polynomials of both the classes of graphs is given by

$$-m \cdot n\,, \tag{14}$$

where m is the number of vertices in individual rings (four for square, three for triangle) and n is the number of rings in the spirograph. For spirographs containing squares, the lowest power in the characteristic polynomial is given by λ^{n+1}. The coefficient of this term is always a multiple of four. In fact, the coefficients of all the terms in the characteristic polynomials of square spirographs are found to be multiples of four.

The pruning method developed in section 2 can be applied to even more complicated spirographs. Consider a class of spirographs which contain hexagons. An example of a linear spirograph containing three hexagons is shown in fig. 5. Suppose h_n

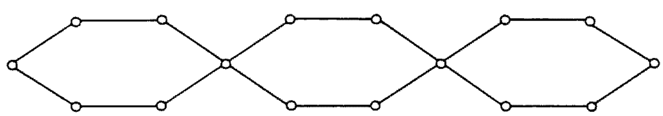


Fig. 5. A linear spirograph which contains three hexagons.

denotes the characteristic polynomials of linear spirographs containing n hexagons. Then recursive relationships can be derived for h_n's for various n's using the pruning method in section 2. Table 4 shows the final characteristic polynomials of linear spirographs containing up to eight hexagons. All the polynomials were derived from simply the characteristic polynomials of a hexagon (C_n) and a linear chain of length five (l_5). The second coefficient of the polynomials for the linear spirographs containing hexagons also follows the same pattern previously discussed. The magnitude of the constant coefficient of the polynomials in table 4 follows the general expression

$$|C| = \begin{cases} 0 & \text{if } n \text{ is even} \\ 4^{n-1} & \text{if } n \text{ is odd.} \end{cases} \tag{15}$$

Further, the constant coefficients alternate in sign for $n = 1, 3, 5, 7$. etc.

Finally, we would like to show that the pruning method is applicable even if there are multiple spiral points in a given ring. As an example of this, consider the spirograph which contains three triangles shown in fig. 6. When the spirograph in this figure is pruned simultaneously at the two spiral points, one obtains the quotient graph Q and two sets of type T in fig. 7. The reduced adjacency matrix A for Q is:

Table 4

Characteristic polynomials of linear spirographs containing hexagons

n	Polynomial
1	$\lambda^6 - 6\lambda^4 + 9\lambda^2 - 4$
2	$\lambda^{11} - 12\lambda^9 + 50\lambda^7 - 92\lambda^5 + 77\lambda^3 - 24\lambda$
3	$\lambda^{16} - 18\lambda^{14} + 127\lambda^{12} - 456\lambda^{10} + 911\lambda^8 - 1034\lambda^6 + 641\lambda^4 - 188\lambda^2 + 16$
4	$\lambda^{21} - 24\lambda^{19} + 240\lambda^{17} - 1312\lambda^{15} + 4338\lambda^{13} - 9080\lambda^{11} + 12\,216\lambda^9 - 10\,448\lambda^7 + 5429\lambda^5 - 1536\lambda^3 + 176\lambda$
5	$\lambda^{26} - 30\lambda^{24} + 389\lambda^{22} - 2876\lambda^{20} + 13\,490\lambda^{18} - 42\,324\lambda^{16} + 91\,298\lambda^{14} - 136\,944\lambda^{12} + 142\,445\lambda^{10} - 100\,830\lambda^8 + 46\,553\lambda^6 - 12\,868\lambda^4 + 1760\lambda^2 - 64$
6	$\lambda^{31} - 36\lambda^{29} + 574\lambda^{27} - 5364\lambda^{25} + 32\,795\lambda^{23} - 138\,800\lambda^{21} + 419\,956\lambda^{19} - 925\,160\lambda^{17} + 1\,496\,871\lambda^{15} - 1\,779\,076\lambda^{13} + 1\,539\,598\lambda^{11} - 950\,500\lambda^9 + 403\,101\lambda^7 - 109\,672\lambda^5 + 16\,736\lambda^3 - 1024\lambda$
7	$\lambda^{36} - 42\lambda^{34} + 795\lambda^{32} - 8\,992\lambda^{30} + 67\,977\lambda^{28} - 364\,190\lambda^{26} + 1\,431\,467\lambda^{24} - 4\,217\,420\lambda^{22} + 9\,436\,331\lambda^{20} - 16\,143\,846\lambda^{18} + 21\,145\,865\lambda^{16} - 21\,113\,992\lambda^{14} + 15\,894\,747\lambda^{12} - 8\,843\,410\lambda^{10} + 3\,517\,489\lambda^8 - 945\,996\lambda^6 + 155\,632\lambda^4 - 12\,672\lambda^2 + 256$
8	$\lambda^{41} - 48\lambda^{39} + 1\,052\lambda^{37} - 13\,976\lambda^{35} + 126\,056\lambda^{33} - 819\,600\lambda^{31} + 3\,982\,684\lambda^{29} - 14\,803\,560\lambda^{27} + 42\,737\,202\lambda^{25} - 96\,770\,336\lambda^{23} + 172\,806\,084\lambda^{21} - 243\,777\,000\lambda^{19} + 271\,009\,936\lambda^{17} - 236\,160\,336\lambda^{15} + 159\,286\,772\lambda^{13} - 81\,642\,776\lambda^{11} + 30\,884\,549\lambda^9 - 8\,233\,168\lambda^7 + 1\,431\,120\lambda^5 - 140\,032\lambda^3 + 5\,376\lambda$

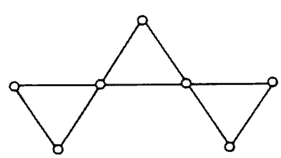
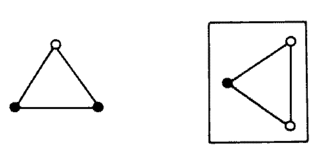


Fig. 6. A linear spirograph containing three triangles.



Q T

Fig. 7. The quotient graph Q and type T (twice) resulting from pruning the graph in fig. 6.

$$\begin{bmatrix} \lambda & -1 & -1 \\ -h_1' & h_1 & -h_1' \\ -h_1' & -h_1' & h_1 \end{bmatrix} \tag{16}$$

The determinant of the above matrix is

$$\lambda(h_1^2 - h_1'^2) - 2h_1' h_1 - 2h_1'^2 . \tag{17}$$

If one substitutes for h_1 and h_1' by the expressions in table 3 for the triangular graphs, one obtains the final polynomial as

$$\lambda((\lambda^3 - 3\lambda - 2)^2 - (\lambda^2 - 1)^2) - 2(\lambda^3 - 3\lambda - 2)(\lambda^2 - 1) - 2(\lambda^2 - 1)^2 . \tag{18}$$

Upon simplification, the above expression yields the characteristic polynomial of the graph in fig. 6 to be

$$\lambda^7 - 9\lambda^5 - 6\lambda^4 + 19\lambda^3 + 20\lambda^2 - 3\lambda - 6 . \tag{19}$$

The proposed method can also be applied to other irregular branched spirographs or circular spirographs. Consider, for example, the triangular spirograph in fig. 8. The characteristic polynomial of this graph can be obtained in two steps of pruning. The simplified expression for the polynomial is:

$$\lambda^{13} - 18\lambda^{11} - 12\lambda^{10} + 115\lambda^9 + 140\lambda^8 - 284\lambda^7 - 536\lambda^6 + 119\lambda^5 + 728\lambda^4$$
$$+ 366\lambda^3 - 156\lambda^2 - 171\lambda - 36. \tag{20}$$

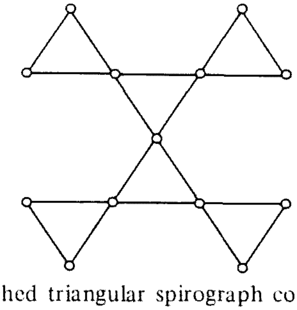


Fig. 8. A branched triangular spirograph containing six rings. For the characteristic polynomial of this graph, see expression (20).

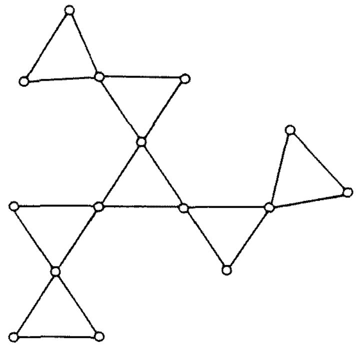


Fig. 9. A branched triangular spirograph containing seven rings. For the characteristic polynomial of this graph, see expression (21).

Consider the branched triangular spirograph in fig. 9. The characteristic polynomial of this spirograph is:

$$\lambda^{15} - 21\lambda^{13} - 14\lambda^{12} + 165\lambda^{11} + 204\lambda^{10} - 549\lambda^{9} - 1026\lambda^{8} + 543\lambda^{7} + 2032\lambda^{6} + 525\lambda^{5} - 1410\lambda^{4} - 885\lambda^{3} + 228\lambda^{2} + 285\lambda + 50. \tag{21}$$

Figure 10 shows a spirograph which contains nine rings. The characteristic polynomial of this graph is:

$$\lambda^{28} - 36\lambda^{26} + 544\lambda^{24} - 4512\lambda^{20} + 22\,496\lambda^{18} - 69\,248\lambda^{16} + 129\,792\lambda^{14} - 140\,288\lambda^{12} + 77\,824\lambda^{10} - 16\,384\lambda^{8}\,. \tag{22}$$

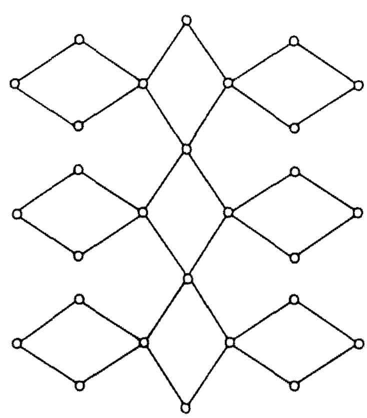


Fig. 10. A branched square spirograph containing nine rings. The characteristic polynomial of this graph is given by (22).

Thus, the pruning method outlined here is applicable for a variety of spirographs, branched, linear, circular, etc. Further applications of spirographs in lattice statistics of Cacti will be considered in a future publication [42].

4. Conclusions

In this investigation, we defined a class of graphs which we called spirographs. A method based on pruning was developed to obtain the characteristic polynomials of spirographs. This method was applied to derive elegant recursive relations for many spirographs. The characteristic polynomials of spirographs containing triangles, squares and hexagons with the number of rings varying from one to ten were obtained. Many of the polynomials are obtained for the first time.

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