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Original Investigations

Analysis of the Topological Dependency of the Characteristic Polynomial in Its Chebyshev Expansion

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The structural dependency (effect of branching and cyclisation) of an alternative form, the Chebyshev expansion, for the characteristic polynomial were investigated systematically. Closed forms of the Chebyshev expansion for an arbitrary star graph and a bicentric tree graph were obtained in terms of the "structure factor" expressed as the linear combination of the "step-down operator". Several theorems were also derived for non-tree graphs. Usefulness and effectiveness of the Chebyshev expansion are illustrated with a number of examples. Relation with the topological index (Z_G) was discussed.

Key words: Characteristic polynomial—Chebyshev polynomial—Topological index—Structure factor—Graph.

1. Introduction

The characteristic polynomial of a graph or structure is one of the important structural invariants, defined as $P_G(x) = (-1)^n \det(A - xE)$; where A and E are, respectively, the adjacency matrix and unit matrix for graph G with n vertices. Recently an alternative but equivalent form for $P_G(x)$ was proposed such that, instead of expressing the polynomial as a function of x, is expressed as a linear combination of the characteristic polynomials $S_n(x)$ of linear chains or paths

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with n points [1]. Let us call this expression as Chebyshev expansion (*vide infra*), which has several simple recurrent properties and has been shown to be useful in constructing the characteristic polynomials for large molecules [2]. Application to selected families of structurally related graphs (molecules) has revealed important regularities in the characteristic polynomials of the individual members of a family which in numerous cases give much simpler pattern than the conventional polynomial form expressed in terms of x.

On the other hand, several new efficient techniques for expanding and solving the characteristic polynomial of complex graphs were proposed quite recently, e.g., the transfer matrix method [3, 4], the partition technique [5], the polynomial matrix method [6–8], the pruning technique [9], the block-diagonalisation method [10], the operator technique [11] etc. The characteristic polynomial is closely related to the topological index Z_G [12, 13] and also to the matching polynomial [14–16], whose interesting mathematical properties have been discussed extensively [17–19]. By combining with some of these new concepts and techniques several important mathematical consequences of the Chebyshev expansion were discovered. These informations are useful not only for obtaining the Hückel molecular orbitals of large π-electron systems but also for elucidating the "topology dependency" of the electronic structure of infinitely large π-electron networks [20].

2. Chebyshev Polynomial

In this paper let the characteristic polynomial of a path graph S_n (i.e., a graph composed of n linearly connected vertices) be denoted as $S_n(x)$ [21], and is expressed as

$$S_n(x)=\sum_{k=0}^{[n/2]}(-1)^k\binom{n-k}{k}x^{n-2k} \qquad (n\geq 0). \tag{1}$$

Unless confusion occurs the notation S_n is used for $S_n(x)$. Incidentally the Chebyshev polynomial of the second kind $S_n(x)$ [22] has been shown to be identical to the characteristic and also the matching polynomials of a path graph S_n [23, 24]. Eq. (1) has already been reported in 1957 by Collatz and Sinogowitz [25], when non-uniqueness of characteristic polynomials was recognised for the first time. From above we have:

$$S_0=1,\quad S_1=x,\quad S_2=x^2-1,\quad S_3=x^3-2x,$$
$$S_4=x^4-3x^2+1,\quad S_5=x^5-4x^3+3x,\quad \text{etc.}$$

By successive substitution for Eq. (1) we get:

$$1=S_0,\quad x=S_1,\quad x^2=S_2+S_0,\quad x^3=S_3+2S_1,$$
$$x^4=S_4+3S_2+2S_0,\quad x^5=S_5+4S_3+5S_1,\quad \text{etc. [26].}$$

Generally x^n is obtained in the form of

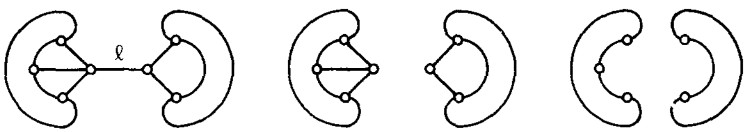
$$x^n = \sum_{k=0}^{[n/2]} B_{n,k} S_{n-2k}. \tag{2}$$

An explicit form of $B_{n,k}$ will be given later.

3. Recurrence Formulae

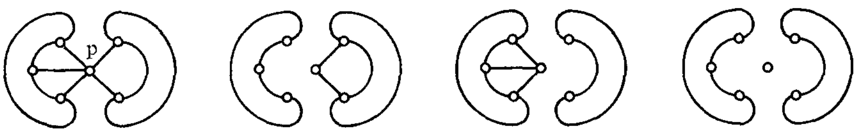
Among the several recurrence formulae for the characteristic polynomials the following two relations are useful:

(I) $P_G(x) = P_{G-l}(x) - P_{G\ominus l}(x)$ [12, 13, 27, 28], (3)



G G−ℓ G⊖ℓ

(II) $P_G(x) = P_{G-\{l_i\}}(x) + P_{G-\{l_j\}}(x) - P_{G-\{l_i+l_j\}}(x)$ [13, 29], (4)



G G−{ℓ$_i$} G−{ℓ$_j$} G−{ℓ$_i$ + ℓ$_j$}

where the meaning of the notations of $\ominus$ and { } is clear from the above diagrams. Note, however, that the pivot edge l in (I) and vertex p in (II) should be so chosen that the original graph G becomes disconnected by their deletion. Application of Eq. (3) to a path graph gives the well-known recurrence formulae for the Chebyshev polynomial of the second kind [12, 23, 30],

$$\begin{aligned} S_n &= S_k \cdot S_{n-k} - S_{k-1} \cdot S_{n-k-1} \qquad (n \geq k \geq 2) \\ S_n &= S_1 \cdot S_{n-1} - S_{n-2} \qquad (n \geq 2). \end{aligned} \tag{5}$$

By successive application of Eq. (5) we obtain [1, 2, 23]:

$$S_m \cdot S_n = S_{m+n} + S_{m+n-2} + S_{m+n-4} + \cdots + S_{|m-n|}. \tag{6}$$

This formula expresses a product of two S functions in terms of the sum of a collection of S functions of the same parity from $m+n$ to $|m-n|$. The formal similarity of Eq. (6) and vector addition of angular momenta can now be exploited by adopting some of the formalism in the algebra of angular momenta, such as the use of step operators. Let us define the following operators $\hat{u}$ and $\hat{d}$ for S_n:

$$\begin{aligned} \hat{u} S_n &= S_{n+1} \qquad (n \geq 0) \\ \hat{d} S_n &= S_{n-1} \qquad (n \geq 1) \end{aligned} \tag{7}$$

or more generally

$$\hat{u}^k S_n = S_{n+k} \qquad (n \geq 0)$$
$$\hat{d}^k S_n = S_{n-k} \qquad (n \geq k), \tag{7'}$$

which represent respectively step-up and step-down operators for S_n. By the use of $\hat{u}$ and $\hat{d}$ we can rewrite some of the previously given recurrence relations and products. For example, with $m = 1$ Eq. (6) becomes:

$$xS_n = S_{n+1} + S_{n-1} = (\hat{u} + \hat{d})S_n \qquad (n \geq 0) \tag{8}$$

or as an operator expression,

$$x = \hat{u} + \hat{d}. \tag{9}$$

With an arbitrary positive integer m Eq. (6) can be expressed as

$$S_m \cdot S_n = (1 + \hat{d}^2 + \hat{d}^4 + \cdots + \hat{d}^{2l})S_{m+n} \qquad (l = \min(m, n)). \tag{10}$$

Further from the definitions of $\hat{u}$ and $\hat{d}$ we have

$$\hat{d}\hat{u} = \hat{u}\hat{d} = 1. \tag{11}$$

Note that Eq. (11) does not hold for the following cases

$$\hat{d}\hat{u}S_0 = S_0 \neq \hat{u}\hat{d}S_0 = 0. \tag{12}$$

From Eqs. (9) and (11) we get

$$\hat{u} = (x + \sqrt{x^2 - 4})/2$$
$$\hat{d} = (x - \sqrt{x^2 - 4})/2. \tag{13}$$

With proper use of the step operators we can now construct the table of $B_{n,k}$ coefficients (Eq. (2)) shown in Table 1, which represents a half-triangle of Pascal, for which the same rules as for Pascal triangle hold, except that the other half

Table 1. $B_{n,k}$ coefficients

n \ k	0	1	2	3	4	5
0	1					
1	1					
2	1	1				
3	1	2				
4	1	3	2			
5	1	4	5			
6	1	5	9	5		
7	1	6	14	14		
8	1	7	20	28	14	
9	1	8	27	48	42	
10	1	9	35	75	90	42

See Eqs. (2) and (16)

of the triangle is suppressed. Note that the series of the coefficients appearing in the last column represent Catalan numbers [31, 32] which can be expressed as:

$$B_{2l,l} = \frac{1}{2l+1}\binom{2l+1}{l}. \tag{14}$$

By observing the following recurrence relations,

$$\begin{aligned} &B_{n,k} = B_{n-1,k-1} + B_{n-1,k} \qquad (1 \le k \le [n/2]) \\ &B_{n,0} = 1, \end{aligned} \tag{15}$$

we get the general expression for $B_{n,k}$ as

$$B_{n,k} = \frac{n-2k+1}{n+1}\binom{n+1}{k}. \tag{16}$$

With the $\hat{d}$ operator, x^n can be expressed as

$$x^n = \sum_{k=0}^{n/2} \frac{n-2k+1}{n+1}\binom{n+1}{k}\hat{d}^{2k}S_n. \tag{17}$$

4. Chebyshev Expansion

By substitution of Eq. (17) into the known forms of the characteristic polynomials expressed in terms of x^k it is straightforward to obtain the equivalent forms, the Chebyshev expansion, of the characteristic polynomials [33]. We can write in general

$$P_G(x) = \sum_{k=0}^{n} c_{G,k}S_{n-k} = S_n + \sum_{k=1}^{n} c_{G,k}S_{n-k}. \tag{18}$$

The explicit forms for the trees of maximal valency four and with not more than nine vertices have been given in the literature [1, 2].

Note that S_{n-k} is expressed as $\hat{d}^kS_n$. Then if we deem a given graph G with n points as a member of a series of graph $\{G_n\}$, we can write Eq. (18) into a compact expression as

$$G_n = \hat{g}S_n \tag{19}$$

with a proper operator $\hat{g}$ of the form

$$\hat{g} = \sum_{k=0}^{m} c_k\hat{d}^k. \tag{20}$$

Let us call $\hat{g}$ as the "structure factor" of the Chebyshev expansion of the characteristic polynomial for the series of graphs $\{G_n\}$, each of which is composed of a "head" in common and a "tail" of different length. Inspection of the available results of the Chebyshev expansion gives us several interesting and useful properties of them, on which we are going to expose as Theorems and Conjectures.

Theorem 1. For a series of graphs $\{G_n\}$, whose characteristic polynomials recur as

$$G_{n+1} = xG_n - G_{n-1}, \tag{21}$$

there exists a common operator $\hat{g}$ of the form of Eq. (20) such that

$$G_n = \hat{g}S_n \tag{19}$$

for n larger than a certain value.

Proof. If two successive entries G_{n-1} and G_n are expressed by a common operator $\hat{g}$ of the form of Eq. (20) with $n-1 \geq m$ as Eq. (19), then by using Eq. (9) we have

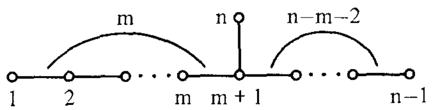
$$\begin{aligned} xG_n &= (\hat{u}+\hat{d})\hat{g}S_n \\ &= \sum_{k=0}^{m} c_k(\hat{u}+\hat{d})\hat{d}^k S_n \\ &= \sum_{k=0}^{m} c_k\hat{d}^k(S_{n+1}+S_{n-1}) \qquad \text{(as long as } n \geq k) \\ &= \hat{g}S_{n+1} + G_{n-1}, \end{aligned}$$

which gives

$$G_{n+1} = \hat{g}S_{n+1}. \qquad \text{(from Eq. (21))} \qquad \text{(Q.E.D.)}$$

5. Star Graphs

As the first example of the Chebyshev expansion consider the following graph G_n,

G_n:  $(n-m-2 \geq m)$

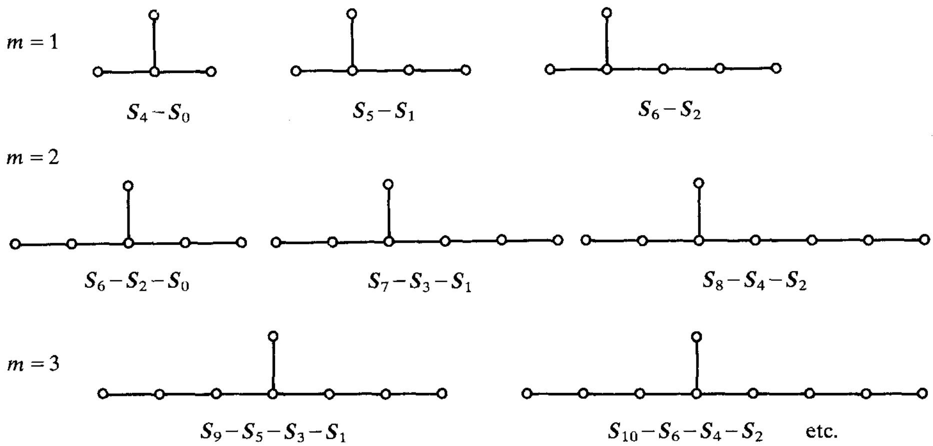
in which a branch of a unit length is attached to the path graph S_{n-1} at the $(m+1)$th point counted from one of the end points of S_{n-1}. Note that the numbering should be done to get the smaller m value, i.e., $m \leq n-m-2$. By choosing this branch as the pivot line l, and using the recurrence formula (I) and Eq. (6), the characteristic polynomial G_n reduces to

$$\begin{aligned} G_n &= S_1 \cdot S_{n-1} - S_m \cdot S_{n-m-2} \\ &= (S_n + S_{n-2}) - (S_{n-2} + S_{n-4} + \cdots + S_{n-2m-2}) \\ &= S_n - S_{n-4} - S_{n-6} - \cdots - S_{n-2m-2}. \end{aligned}$$

Now the structure factor, or operator g, for G_n in this case is

$$\begin{aligned} \hat{g} &= 1 - \hat{d}^4(1 + \hat{d}^2 + \hat{d}^4 + \cdots + \hat{d}^{2m-2}) \\ &= 1 - D_1 \cdot D_m. \end{aligned} \tag{22}$$

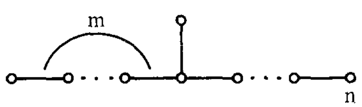
Table 2. The Chebyshev expansions for the characteristic polynomials of the lower members of graphs with a branch of unit length



The structure factor

$$\hat{g} = 1 - \hat{d}^4(1 + \hat{d}^2 + \cdots + \hat{d}^{2m-2})$$
$$= 1 - D_1 \cdot D_m$$

G_n:



The notation

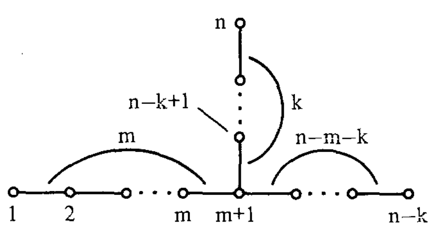
$$D_m = \hat{d}^2 + \hat{d}^4 + \cdots + \hat{d}^{2m} \tag{23}$$

will be useful for discussing the structure factor for complicated graphs.

One can observe in Table 2 the regularity of the Chebyshev expansion of the characteristic polynomials for the lower members of the above series of graphs [35]. Generalisation of this result is straightforward and worth stating as a Theorem.

Theorem 2. The structure factor for the following graph G_n

G_n:



$\begin{pmatrix} n \geq 2k + 2m \\ m \geq k \end{pmatrix}$ [38]

is given by

$$\hat{g} = 1 - D_m \cdot D_k. \tag{24}$$

Proof. Choose the line joining the points $m+1$ and $n-k+1$ as the pivot, and we get

$$G_n = S_k \cdot S_{n-k} - S_{k-1} \cdot S_m \cdot S_{n-m-k-1}$$

$$= (S_k \cdot S_{n-k} - S_{k-1} \cdot S_{n-k-1}) - S_{k-1}(S_{n-k-3} + \cdots + S_{n-k-2m-1}) \quad (\text{assume } n-m-k-1 \geq m)$$

$$= S_n - S_{k-1}(S_{n-k-3} + S_{n-k-5} + \cdots + S_{n-k-2m-1}) \quad (\text{from Eq. (5)})$$

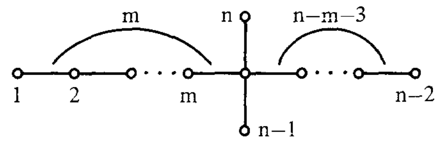
$$= S_n - (1 + \hat{d}^2 + \cdots + \hat{d}^{2k-2})(S_{n-4} + S_{n-6} + \cdots + S_{n-2m-2})$$

$$(\text{assume } n-k-2m-1 \geq k-1 \text{ and from Eq. (10)})$$

$$= S_n - (1 + \hat{d}^2 + \cdots + \hat{d}^{2k-2})(1 + \hat{d}^2 + \cdots + \hat{d}^{2m-2})S_{n-4}$$

$$= (1 - D_k \cdot D_m)S_n. \qquad \text{(Q.E.D.)}$$

Next consider the following graph G_n,

G_n:  $(n-m-3 \geq m)$

in which two branches of unit length are attached to the $(m+1)$th point counted from the nearest end point of S_{n-2}. By choosing one of the branches as the pivot line l we get

$$G_n = S_1(1 - \hat{d}^2 D_m)S_{n-1} - S_1 \cdot S_m \cdot S_{n-m-3} \quad (\text{from Eqs. (3) and (22)})$$

$$= (\hat{u} + \hat{d})\{(1 - \hat{d}^2 D_m)\hat{d} - (1 + \hat{d}^2 + \cdots + \hat{d}^{2m})\hat{d}^3\}S_n$$

$$= (1 + \hat{d}^2)\{(1 - \hat{d}^2 D_m) - \hat{d}^2(1 + D_m)\}S_n$$

$$= (1 + \hat{d}^2)(1 - \hat{d}^2 - 2\hat{d}^2 D_m)S_n.$$

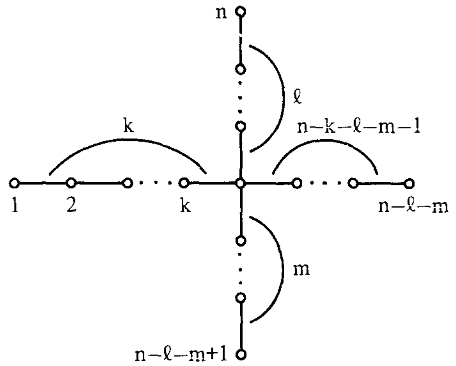
This expression can be rearranged into the following form in line with the result of more general cases.

$$\hat{g} = (1 - D_1 \cdot D_m)^2 - D_1^2(1 + D_m)^2. \tag{25}$$

Further, by extending the lengths of both branches one by one we get the following Theorem.

Theorem 3. The structure factor for the following graph G_n

G_n:



$n \geq 2(k+l+m)-1$

is given by

$$\hat{g}=(1-D_k \cdot D_l)(1-D_k \cdot D_m)-D_l \cdot D_m(1+D_k)^2 \tag{26}$$

$$=1-(D_k \cdot D_l+D_k \cdot D_m+D_l \cdot D_m)-2D_k \cdot D_l \cdot D_m. \tag{27}$$

Examples of Theorem 3 for the series of graphs with $k=l=3$, $m=2$ are given in Table 3. Application of Theorem 3 to these graphs gives

$$\hat{g}=1-3\hat{d}^4-8\hat{d}^6-13\hat{d}^8-14\hat{d}^{10}-11\hat{d}^{12}-6\hat{d}^{14}-2\hat{d}^{16} \tag{28}$$

which is valid for the graphs with $n \geq 15$, while the recurrence formula

$$G_{n+2}=xG_{n+1}-G_n \tag{21'}$$

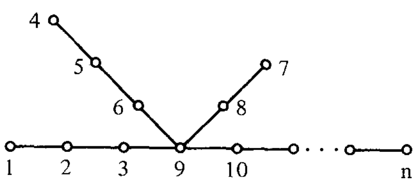
holds for the graphs as low as $n=9$. This discrepancy arises from the inequality (12).

Generalisation of Theorem 2 and 3 gives the following interesting Conjecture for an arbitrary star graph.

Table 3. Examples of Theorem 3 on the characteristic polynomial and its Chebyshev expansion

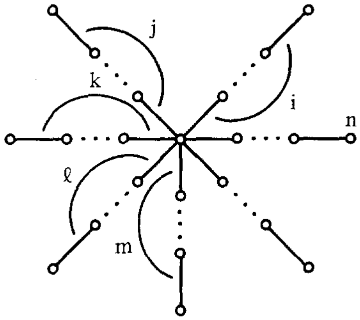
$n=14$	$G_{14}=x^{14}-13x^{12}+63x^{10}-146x^8+169x^6-90x^4+16x^2$
	$=S_{14}-3S_{10}-8S_8-13S_6-14S_4-11S_2-\underline{4S_0}$
$n=15$	$G_{15}=x^{15}-14x^{13}+75x^{11}-198x^9+273x^7-188x^5+54x^3-4x$
	$=S_{15}-3S_{11}-8S_9-13S_7-14S_5-11S_3-6S_1$
$n=16$	$G_{16}=x^{16}-15x^{14}+88x^{12}-261x^{10}+419x^8-357x^6+144x^4-20x^2$
	$=S_{16}-3S_{12}-8S_{10}-13S_8-14S_6-11S_4-6S_2-2S_0$
$n=17$	$G_{17}=x^{17}-16x^{15}+102x^{13}-336x^{11}+617x^9-630x^7+332x^5-74x^3+4x$
	$=S_{17}-3S_{13}-8S_{11}-13S_9-14S_7-11S_5-6S_3-2S_1$

G_n:



Note that the underlined term in G_{14} does not obey Eq. (28)

Theorem 4 (Conjecture). The structure factor for the following star graph G_n with a sufficient length of the tail

G_n: 

$(n \geq 2(i+j+k+l+m\ldots)-1)$

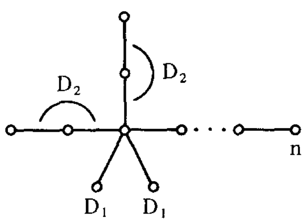
is given by

$$\hat{g} = 1 - \sum_{i<j} D_i \cdot D_j - 2 \sum_{i<j<k} D_i \cdot D_j \cdot D_k$$

$$-3 \sum_{i<j<k<l} D_i \cdot D_j \cdot D_k \cdot D_l - 4 \sum_{i<j<k<l<m} D_i \cdot D_j \cdot D_k \cdot D_l \cdot D_m - \cdots. \tag{29}$$

This expression can be deemed as an extension of Eq. (27) in Theorem 3. Although we do not yet get a rigorous proof of this Theorem, its validity has been checked by a number of examples as shown in Table 4. Of course, this Theorem is not necessary for the calculation of the Hückle MO of conjugated hydrocarbons, but it is very important for discussing the relationship between the branching of a tree and the coefficients of the characteristic polynomial. For example, we can derive quite readily the following Collorary.

Table 4. Example of Theorem 4

G_n: 

$$\hat{g} = 1 - (D_1^2 + 4D_1D_2 + D_2^2) - 2(2D_1^2D_2 + 2D_1D_2^2) - 3D_1^2D_2^2$$
$$= 1 - 6\hat{d}^4 - 14\hat{d}^6 - 16\hat{d}^8 - 10\hat{d}^{10} - 3\hat{d}^{12}$$

$n=10$	$G_{10} = x^{10} - 9x^8 + 22x^6 - 19x^4 + 5x^2$ $= S_{10} - 6S_6 - 14S_4 - 16S_2 - \underline{7S_0}$	$D_1 = \hat{d}^2$ $D_2 = \hat{d}^2 + \hat{d}^4$
$n=11$	$G_{11} = x^{11} - 10x^9 + 30x^7 - 34x^5 + 15x^3 - 2x$ $= S_{11} - 6S_7 - 14S_5 - 16S_3 - 10S_1$	
$n=12$	$G_{12} = x^{12} - 11x^{10} + 39x^8 - 56x^6 + 34x^4 - 7x^2$ $= S_{12} - 6S_8 - 14S_6 - 16S_4 - 10S_2 - 3S_0$	

The graphs with $n \leq 10$ does not obey the above structure factor $\hat{g}$. See the underlined term in G_{10}

Collorary. The structure factor for a star graph, i.e., a tree with a single branch point, does not contain any step-up operator. That is all the coefficients c_k's ($k \geq 0$) of the Chebyshev expansion for a star graph are negative.

6. Bicentric Tree Graphs

Now try to examine the tree graphs with two branch points. If two branch points are separated to a reasonable extent an interesting property can be observed.

Theorem 5. If two "structures" (branching and/or cyclisation) at both the ends of a long chain are separated well, the structure factor of this graph is the product of those for the component structures.

Proof. Consider two graphs F_k and G_l with the structure factors of f and g such that

$$F_k = \hat{f}S_k$$
$$G_l = \hat{g}S_l, \tag{30}$$

and construct graph H_{k+l} by joining both their tail ends (see Fig. 1). Further assume that the two relations (30) hold at least for the next lower members of F_k and G_l, namely,

$$F_{k-1} = \hat{f}S_{k-1}$$
$$G_{l-1} = \hat{g}S_{l-1}. \tag{30'}$$

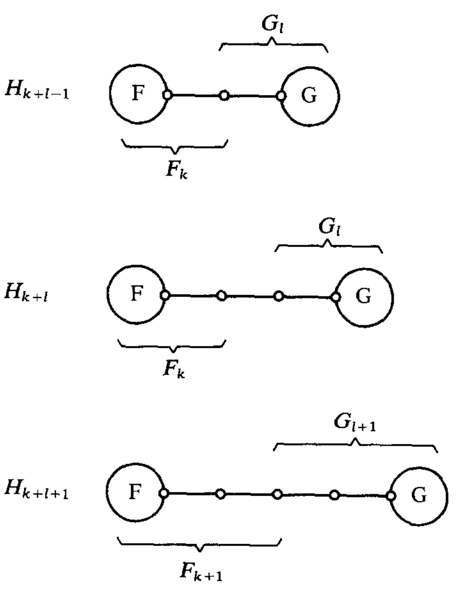


Fig. 1. A series of graphs composed of two "structures" F_k and G_l

Then by the use of the recurrence relation (I) we have

$$\begin{aligned} H_{k+l} &= F_k \cdot G_l - F_{k-1} \cdot G_{l-1} \\ &= \hat{f}S_k \cdot \hat{g}S_l - \hat{f}S_{k-1} \cdot \hat{g}S_{l-1} \\ &= \hat{f}(S_k\hat{g}S_l - S_{k-1}\hat{g}S_{l-1}). \end{aligned}$$

Now $\hat{g}$ is expressed in terms of the operator $\hat{d}$ as in Eq. (20). Then we have

$$\begin{aligned} S_k\hat{g}S_l - S_{k-1}\hat{g}S_{l-1} &= \sum_{j=0}^{m} c_j(S_k\hat{d}^jS_l - S_{k-1}\hat{d}^jS_{l-1}) \\ &= \sum_{j=0}^{m} c_j(S_k \cdot S_{l-j} - S_{k-1} \cdot S_{l-j-1}) \qquad \text{(as long as } l-1 \geq j\text{)} \\ &= \sum_{j=0}^{m} c_jS_{k+l-1} \qquad \text{(from Eq. (5))} \\ &= \sum_{j=0}^{m} c_j\hat{d}^jS_{k+l} \\ &= \hat{g}S_{k+l}. \end{aligned}$$

Thus we get

$$H_n = \hat{f}\hat{g}S_n \qquad (n = k + l). \tag{31}$$

Collorary: The characteristic polynomials of the series of graphs $\{H_n\}$ generated by successive insertion of lines between the two structures of F_k and G_l (see Fig. 1) recur as

$$H_{n+1} = xH_n - H_{n-1}.$$

Proof. Application of relations (I) and (II) to the series of graphs H_{k+l} gives

$$H_{k+l} = F_k \cdot G_l - F_{k-1} \cdot G_{l-1} \tag{32}$$

$$H_{k+l-1} = F_{k-1} \cdot G_l + F_k \cdot G_{l-1} - xF_{k-1} \cdot G_{l-1} \tag{33}$$

$$H_{k+l+1} = F_{k+1} \cdot G_l + F_k \cdot G_{l+1} - xF_k \cdot G_l. \tag{34}$$

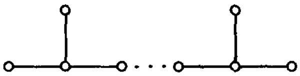
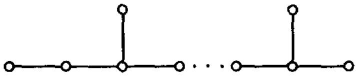
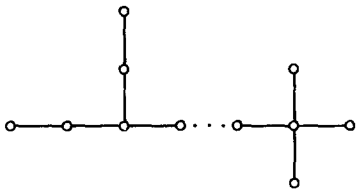
By combining the first two equations (32) and (33) we get

$$\begin{aligned} xH_{k+l} - H_{k+l-1} &= xF_k \cdot G_l - F_{k-1} \cdot G_l - F_k \cdot G_{l-1} \\ &= (xF_k - F_{k-1})G_l + F_k(xG_l - G_{l-1}) - xF_k \cdot G_l \\ &= F_{k+1} \cdot G_l + F_k \cdot G_{l+1} - xF_k \cdot G_l \qquad \text{(from Eq. (4) or (21))} \\ &= H_{k+l+1}. \qquad \text{(from Eq. (34))} \end{aligned}$$

(Q.E.D.)

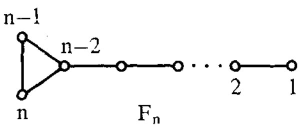
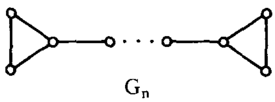
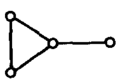
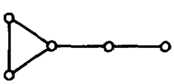
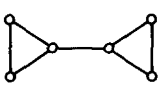
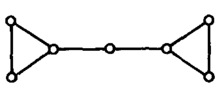
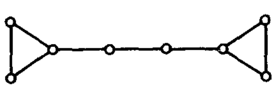
How Theorem 5 and its Collorary hold for bicentric graphs can be seen in Table 5. Note that these Theorems hold also for the cases where F_k and/or G_l contain non-tree structures. Examples are shown in Table 6.

Table 5. Examples of Theorem 5 and its Collorary

G_n	$\hat{g}$	[a]	[b]
	$(1-\hat{d}^4)^2 = 1-2\hat{d}^4+\hat{d}^8$	7	7
	$(1-\hat{d}^4)(1-\hat{d}^4-\hat{d}^6)$ $= 1-2\hat{d}^4-\hat{d}^6+\hat{d}^8+\hat{d}^{19}$	9	8
	$(1-\hat{d}^4-2\hat{d}^6-\hat{d}^8)(1-3\hat{d}^4-2\hat{d}^6)$ $= 1-4\hat{d}^4-4\hat{d}^6+2\hat{d}^8+8\hat{d}^{10}+7\hat{d}^{12}+2\hat{d}^{14}$	13	10

[a] Minimum n for satisfying the common structure factor $\hat{g}$
[b] Minimum n for satisfying the recurrence relation $G_{n+1} = xG_n - G_{n-1}$

Table 6. Examples of Theorem 5 and its Collorary to non-tree graphs

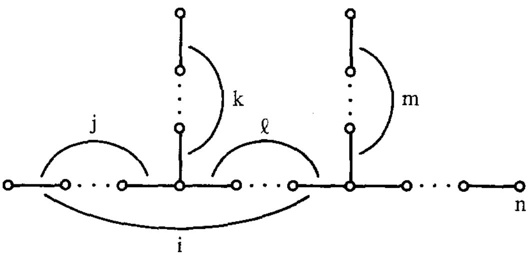
		$\hat{f} = 1-\hat{d}^2-2\hat{d}^3-\hat{d}^4 \quad (n \geq 4)$
		$\hat{g} = \hat{f}^2 = 1-2\hat{d}^2-4\hat{d}^3-\hat{d}^4+4\hat{d}^5$ $+6\hat{d}^6+4\hat{d}^7+\hat{d}^8 \quad (n \geq 7)$
F_n		$F_4 = x^4-4x^2-2x+1 = S_4-S_2-2S_1-S_0$
		$F_5 = x^5-5x^3-2x^2+4x+2$ $= S_5-S_3-2S_2-S_1$
G_n		$G_6 = x^6-7x^4-4x^3+11x^2+12x+3$ $= S_6-2S_4-4S_3-S_2+4S_1-S_0$
		$G_7 = x^7-8x^5-4x^4+17x^3+16x^2-2x-4$ $= S_7-2S_5-4S_4-S_3+4S_2+6S_1+4S_0$
		$G_8 = x^8-9x^6-4x^5+24x^4+20x^3-13x^2-16x-3$ $= S_8-2S_6-4S_5-S_4+4S_3+6S_2+4S_1+S_0$

Note that although G_6 does not obey the structure factor $\hat{g}$ the following recurrence relation holds: $G_8 = xG_7 - G_6$

If the two branch points get closer, both the effects of branching on the characteristic polynomial interact with each other. Inspection of the Chebyshev expansions for a number of bicentric graphs yields the following Conjecture.

Theorem 6 (Conjecture). For a graph G_n with two branch points and a sufficiently long tail as

G_n:

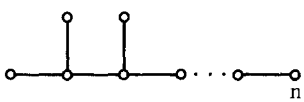
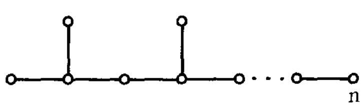
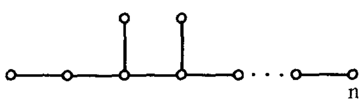
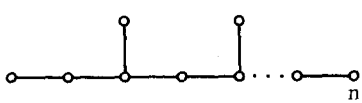
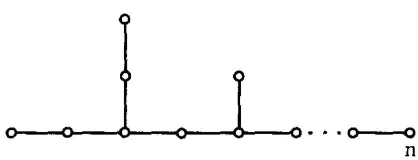


the structure factor is given by

$$\hat{g} = (1 - D_i \cdot D_m)(1 - D_j \cdot D_k) - \hat{d}^{2l} D_k \cdot D_m (1 + D_j)^2 \tag{35}$$

$$= 1 - (D_i \cdot D_m + D_j \cdot D_k + \hat{d}^{2l} D_k \cdot D_m) - 2\hat{d}^{2l} D_j \cdot D_k \cdot D_m + D_j \cdot D_k \cdot D_l \cdot D_m. \tag{36}$$

Table 7. Examples of Theorem 6

G_n	$\hat{g}^a$
	$(1-D_1^2)(1-D_1 \cdot D_2)-\hat{d}^2 D_1^2(1+D_1)^2$ $=1-2\hat{d}^4-2\hat{d}^6-\hat{d}^8$ $(n \geq 7)$
	$(1-D_1^2)(1-D_1 \cdot D_3)-\hat{d}^4 D_1^2(1+D_1)^2$ $=1-2\hat{d}^4-\hat{d}^6-\hat{d}^8-\hat{d}^{10}$ $(n \geq 9)$
	$(1-D_1 \cdot D_2)(1-D_1 \cdot D_3)-\hat{d}^2 D_1^2(1+D_2)^2$ $=1-2\hat{d}^4-3\hat{d}^6-2\hat{d}^8-\hat{d}^{10}$ $(n \geq 9)$
	$(1-D_1 \cdot D_2)(1-D_1 \cdot D_4)-\hat{d}^4 D_1^2(1+D_2)^2$ $=1-2\hat{d}^4-2\hat{d}^6-\hat{d}^8-\hat{d}^{10}-\hat{d}^{12}$ $(n \geq 11)$
	$(1-D_2^2)(1-D_1 \cdot D_4)-\hat{d}^4 D_1 \cdot D_2(1+D_2)^2$ $=1-2\hat{d}^4-3\hat{d}^6-2\hat{d}^8-\hat{d}^{10}-\hat{d}^{12}-\hat{d}^{14}$ $(n \geq 13)$

[a] $D_m = \hat{d}^2 + \hat{d}^4 + \cdots + \hat{d}^{2m}$

In Table 7 are given several examples of Theorem 6. No rigorous proof can be reached at the present time, but its validity has been checked extensively. Note that if we put $l = 0$ and $D_l = 0$ into Eqs. (35) and (36) we get Eqs. (26) and (27), respectively.

Although we have not yet obtained a general expression of the Chebyshev expansion for an arbitrary tree graph, the regularity of the branching effect on this expansion reminds one of that of the topological index, Z_G, proposed by one of the present authors [12]. It will be shown that by the use of the non-adjacent numbers and topological index [39] we can analyse more rigorously the relationship between the topological structure (i.e., branching and cyclisation) and the coefficients of the Chebyshev expansion. Through this relationship the structure dependency of the (conventional) characteristic polynomial of a graph will be clarified.

7. Non-adjacent Number and Topological Index

The non-adjacent number $p(G, k)$ is defined as the number of ways for choosing k disconnected lines from graph G, with $p(G, 0)$ being defined as a unity [12]. The topological index Z_G is the sum of all the $p(G, k)$ numbers for G:

$$Z_G = \sum_{k=0}^{m} p(G, k), \tag{37}$$

and was found to be correlated with a number of chemical problems, such as thermodynamic properties of saturated hydrocarbons [40, 41], Hückel molecular orbital energies [42] and bond orders [43, 44] for unsaturated hydrocarbons, coding and classification of the molecular structure [45], etc. For tree graphs it was shown [12] that the characteristic polynomial $P_G(x)$ can be expressed in terms of the non-adjacent numbers as follows:

$$P_G(x) = \sum_{k=0}^{[n/2]} (-1)^k p(G, k) x^{n-2k}. \tag{38}$$

For a non-tree graph G with n points we need some "ring corrections" as [13, 44]

$$P_G(x) = \sum_{k=0}^{[n/2]} (-1)^k p(G, k) x^{n-2k} + \sum_{i}^{G \supseteq R_i} (-2)^{r_i} \sum_{k=0}^{m} (-1)^k p(G \ominus R_i, k) x^{n-n_i-2k} \tag{39}$$

where the second term is the sum of the contributions of all the component rings R_i together with all the possible combinations of r_i disjoint rings, and n_i is the number of points in R_i, a ring or a set of rings.

Suppose a graph G with n points, m_3 triangles, m_4 tetragons, and m_r independent rings. Here m_r is the minimum number of lines to be deleted for getting a tree and called as a cyclomatic number or the first Betti number [46]. By close inspection of Eq. (39) it can be shown that the coefficients of the higher orders of $P_G(x)=\sum a_k x^{n-k}$ is expressed in terms of these numbers as

$$a_0=1, \quad a_1=0, \quad a_2=-(m_r+n-1), \quad a_3=-2m_3, \quad a_4=p(G,2)-2m_4, \tag{40}$$

while the lower coefficients become involved. Then by using relations (2), (16), and (40) we get the following Theorem.

Theorem 7. The higher terms of the Chebyshev expansion of a graph is given by

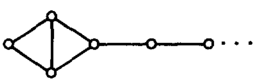
$$P_G(x)=S_n-m_rS_{n-2}-2m_3S_{n-3} -[(n-3)\{(n-2)/2+m_r\}+2m_4-p(G,2)]S_{n-4}-\cdots \tag{41}$$

or

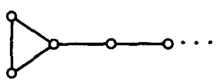
$$\hat{g}=1-m_r\hat{d}^2-2m_3\hat{d}^3-[(n-3)\{(n-2)/2+m_r\}+2m_4-p(G,2)]\hat{d}^4-\cdots. \tag{41'}$$

As has already been noted that the Chebyshev expansion of a tree graph is in the form of $S_n-aS_{n-4}-\cdots$ $(a\geq 0)$, while the coefficients of the S_{n-2} and S_{n-3} terms give the cyclomatic number and the number of triangles, respectively. For tree graphs further inspection of the expansion coefficients will be given in the later discussion.

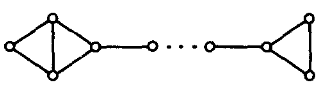
Examples of Theorem 7 are given in Table 8. Note that the structure factor for the last entry in Table 8 can be obtained as the product of those for the component structures as predicted by Theorem 5 as



$$\hat{f}=1-2\hat{d}^2-4\hat{d}^3-4\hat{d}^4-2\hat{d}^5-\hat{d}^6 \qquad (n\geq 6)$$



$$\hat{g}=1-\hat{d}^2-2\hat{d}^3-\hat{d}^4 \qquad (n\geq 6)$$



$$\hat{f}\hat{g}=1-3\hat{d}^2-6\hat{d}^3-3\hat{d}^4+6\hat{d}^5+13\hat{d}^6 +14\hat{d}^7+9\hat{d}^8+4\hat{d}^9+\hat{d}^{10}. \qquad (n\geq 9)$$

The relation between the branching and the coefficients of the Chebyshev expansion is clear for tree graphs.

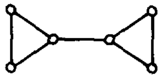
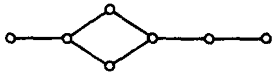
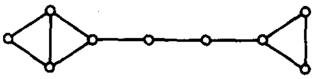
Theorem 8. If the decrement $\delta p(G,k)$ of the $p(G,k)$ number for a tree graph $G_n\equiv G$ relative to the isomeric path graph S_n is defined as

$$\delta p(G,k)=p(S_n,k)-p(G,k), \tag{42}$$

the Chebyshev expansion for G is given by

$$P_G(x)=\sum_{l=0}^{[n/2]}\left(\sum_{k=0}(-1)^k B_{n-2k,l-k}\,p(G,k)\right)S_{n-2l} \tag{43}$$

Table 8. Example of Theorem 7

G	n	m_r	m_3	m_4	$p(G,2)$	$P_G(x)$
	6	2	2	0	11	$S_6-2S_4-4S_3-S_2+4S_1-S_0$
	7	1	0	1	12	$S_7-S_5-4S_3-3S_1$
	9	3	3	1	38	$S_9-3S_7-6S_6-3S_5+6S_4+13S_3+14S_2+9S_1+4S_0$

The terms over the wavy line can directly be obtained from Theorem 7, to which all the notations are referred

or

$$P_G(x)=S_n-\sum_{l=2}^{[n/2]}\left(\sum_{k=2}^{l}(-1)^k B_{n-2k,l-k}\delta p(G,k)\right)S_{n-2l}. \tag{44}$$

Proof. By putting Eq. (2) into Eq. (38) we get

$$P_G(x)=\sum_{k=0}^{m}(-1)^k p(G,k)\sum_{j=0}^{m-k}B_{n-2k,j}S_{n-2k-2j},$$

where $m=[n/2]$. If we introduce another subscript $j=l-k$, the double summation in the above equation can be converted into

$$\sum_{k=0}^{m}\sum_{j=0}^{m-k}\equiv\sum_{l=0}^{m}\sum_{k=0}^{l} \tag{45}$$

to give Eq. (43). By using the relations (42) Eq. (43) is splitted into two parts as

$$P_G(x)=\sum_{l=0}^{m}\left\{\sum_{k=0}^{l}(-1)^k B_{n-2k,l-k}\binom{n-k}{k}\right.$$
$$\left.-\sum_{k=0}^{l}(-1)^k B_{n-2k,l-k}\delta p(G,k)\right\}S_{n-2l}. \tag{46}$$

As will be proved in Appendix there is a novel identity as

$$\sum_{k=0}^{l}(-1)^k B_{n-2k,l-k}\binom{n-k}{k}=\begin{cases}1 & l=0\\ 0 & l>0\end{cases}. \tag{47}$$

For tree graphs $\delta p(G,1)=0$ and for all graphs $\delta p(G,0)=0$. Then Eq. (46) reduces to Eq. (44). (Q.E.D.)

At first sight Eqs. (43) and (44) look alike. However, the latter gives us a deeper information on the structural features of the tree graph. That is the lower terms of Eq. (44) can be written down as

$$P_G(x) = S_n - \delta p(G,2)S_{n-4} - \{(n-5)\delta p(G,2) - \delta p(G,3)\}S_{n-6}$$
$$- \{(n-4)(n-7)\delta p(G,2)/2 - (n-7)\delta p(G,3) + \delta p(G,4)\}S_{n-8} - \cdots . \quad (48)$$

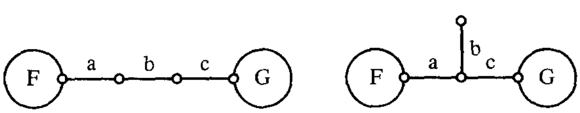
The coefficients of the S_{n-4} term, $\delta p(G, 2)$, is known to be obtained by adding the contributions from different modes of branching as [12, 41]

$$p(G,2) = (\mathrm{Y}) + 3(\mathrm{X}),$$

where (Y) and (X) respectively represent the numbers of points the degree of which is three (tertiary) and four (quaternary). The reason why the tertiary and quaternary points have the $\delta p(G, 2)$ contributions of one and three will be clear from Fig. 2. Note that in the argument in Fig. 2 both the terminal structures, F and G, are irrelevant. Thus the effect of branching on the $p(G, k)$ numbers is

a) Tertiary branching

Entry to the $p(G, 2)$ number?

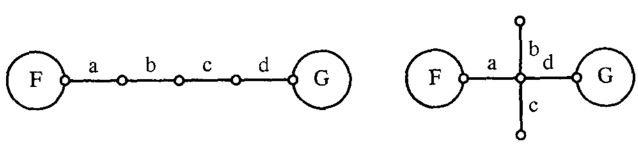


pair of lines	S_n	$G_n \equiv G$
a–b	no	no
a–c	yes	no
b–c	no	no

$$\delta p(G,2) = p(S_n, 2) - p(G,2) = 1$$

b) Quaternary branching

Entry to the $p(G, 2)$ number?



pair of lines	S_n	$G_n \equiv G$
a–b	no	no
a–c	yes	no
a–d	yes	no
b–c	no	no
b–d	yes	no
c–d	no	no

$$\delta p(G,2) = p(S_n, 2) - p(G,2) = 3$$

Fig. 2. Diagram illustrating the decrement $\delta p(G, 2)$ of the non-adjacent number at the tertiary and quaternary points

additive. By extending this discussion [47] one can infer that

$$\delta p(G,2) = \sum_{m=3} \binom{m-1}{2} \text{(number of points of degree } m\text{)}. \tag{49}$$

A number of mathematical relations were found between the structure and the topological index (the sum of $p(G, k)$ numbers) in connection with the theoretical interpretation of the empirical rules on the thermodynamic properties such as boiling point and absolute entropy [12, 40, 41]. By the aid of the theories developed here on the Chebyshev expansion these problems can be treated and solved in a unified manner.

8. Cyclic Graphs

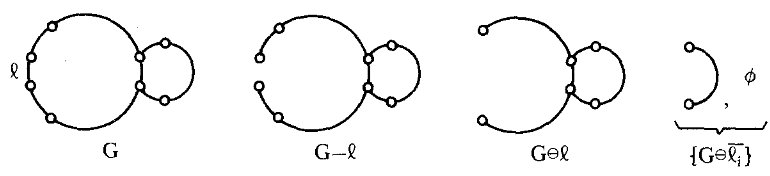
For a cycle graph C_n with n points the characteristic polynomial can be expressed in terms of S_n:

$$C_n(x) = C_n = S_n - S_{n-2} - 2S_0$$

$$= \sum_{k=0}^{n/2} (-1)^k \frac{n}{n-k} \binom{n-k}{k} x^{n-2k} - 2. \quad [12] \tag{50}$$

Note that in this case the expression $C_n(x)$ differs from the Chebyshev polynomial of the second kind [22], where the last term in Eq. (50) is missing [48]. The relation (50) does neither follow from the recurrence relation (I) nor (II) but from another recurrence relation [44]. Namely,

$$\text{(III)} \quad P_G(x) = P_{G-l}(x) - P_{G\ominus l}(x) - 2\sum_i P_{G\ominus \bar{l}_i}(x), \tag{51}$$

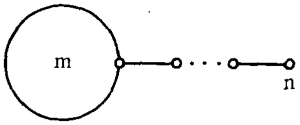
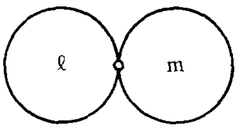
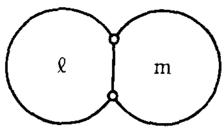


where $\bar{l}_i$ means a detour path from the one end of l to another end, and the contributions from all such possible paths are to be taken. This relation holds for all the cases, and the relation (I) is a special case of (III).

The Chebyshev expansion for substituted C_n cycles becomes more involved, but just as in the case of branched chains for a family of structurally related systems one can recognise regularity in the coefficients of the Chebyshev expansion and derive general expressions, selected examples of which are shown in Table 9.

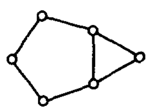
The general expressions for these series of graphs can easily be derived by using the recurrence relations (I)–(III), (10), and (50). As the last example of the utility

Table 9. Structural factors for some series of cyclic graphs

G_n	$\hat{g}$ [a]	Remark
	$1-\hat{d}^2-\hat{d}^4-\cdots-\hat{d}^{2m-2}-2\hat{d}^m$ $=1-D_{m-1}-2\hat{d}^m$	$n \geq [3m/2]$
	$1-2\hat{d}^2-2\hat{d}^4-\cdots-2\hat{d}^{2m-2}-\hat{d}^{2m}-2\hat{d}^m-2\hat{d}^l$ $=1-2D_{m-1}-\hat{d}^{2m}-2\hat{d}^m-2\hat{d}^l$	$l \geq m$ $n=l+m-1$
	$1-2\hat{d}^2-\hat{d}^4-\hat{d}^6-\cdots-\hat{d}^{2m-2}-2\hat{d}^m-2\hat{d}^l-2\hat{d}^n$ $=1-D_{m-1}-\hat{d}^2-2\hat{d}^m-2\hat{d}^l-2\hat{d}^n$	$l \geq m$ $n=l+m-2$

[a] $D_m = \hat{d}^2+\hat{d}^4+\cdots+\hat{d}^{2m}$

of the Chebyshev expansion let us consider the following graph



The structure factor for this graph is readily obtained by using the results in Table 9 as

$$\hat{g} = 1-2\hat{d}^2-2\hat{d}^3-\hat{d}^4-2\hat{d}^5-2\hat{d}^6,$$

giving

$$P_G(x) = x^6-7x^4-2x^3+11x^2+2x-4.$$

The coefficients of the second and third terms of both the expressions reveal to us that the graph has two rings one of which is a triangle (see Theorem 7).

9. Concluding Remarks

We have illustrated and exposed the Theorems of the alternative form for the characteristic polynomial for several families of structurally related molecular skeletons expressed in terms of the Chebyshev polynomials. The novel forms show considerable simplicity and allow deduction of general forms with fewer initial members of a family. In addition, the recurrent expression for characteristic polynomials of a family can be proved valid for higher members, thus avoiding constructions for large related structures. While mathematically equivalent, the regrouping of terms makes patterns for coefficients more obvious in many instances, and in addition their interpretation somewhat different from that of a_k coefficients. By focusing attention on families of graphs, rather than individual members one arrives at possible characterisation of graphs via the characteristic polynomial, in which one associated with a graph its family expression and the corresponding n. While some graphs can simultaneously be members of different families, some pairs of graphs of different structures may have the same characteristic polynomial and are called isospectral [49]. The Chebyshev expansion of the characteristic polynomials for these series of graphs may potentially be useful for the analysis of these problems.

Appendix

Proof of Eq. (47).

We know two relations (1) and (2) between $S_n(x)$ and x^n,

$$S_n(x) = \sum_{k=0}^{m} (-1)^k \binom{n-k}{k} x^{n-2k} \tag{1}$$

and

$$x^p = \sum_{j=0}^{[p/2]} B_{p,j} S_{p-2j}, \tag{2}$$

with $m = [n/2]$. If we put $p = n - 2k$ and introduce another subscript $j = l - k$, the summation of j from 0 to $[p/2]$ is transformed to that of l from k to m. Then Eq. (2) becomes

$$x^{n-2k} = \sum_{l=k}^{m} B_{n-2k,l-k} S_{n-2l}. \tag{2'}$$

Substitution of Eq. (2') into Eq. (1) yields

$$\begin{aligned} S_n(x) &= \sum_{k=0}^{m} \sum_{l=k}^{m} (-1)^k B_{n-2k,l-k} \binom{n-k}{k} S_{n-2l} \\ &= \sum_{l=0}^{m} \sum_{k=0}^{l} (-1)^k B_{n-2k,l-k} \binom{n-k}{k} S_{n-2l}, \end{aligned} \tag{A}$$

where the order and the direction of the double summation have been changed. In order for Eq. (A) to be satisfied for all l, the following equality should be obeyed:

$$\sum_{k=0}^{l} (-1)^k B_{n-2k,l-k} \binom{n-k}{k} = \begin{cases} 1 & l=0 \\ 0 & l>0 \end{cases}$$

which is nothing else but Eq. (47).

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