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Properties of "structure factor" of characteristic polynomial and a proof of Hosoya–Randić conjectures

He Wenchen[1] **and He Wenjie**[2]

[1] Hebei Chemical Engineering Institute, Yu Hua Road, Shijiazhuang, China
[2] Hebei Academy of Sciences, You Yi Street, Shijiazhuang, China

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Some properties of "structure factor" of characteristic polynomial are discussed and Hosoya-Randić conjectures are proved rigorously.

Key words: Characteristic polynomial — Chebyshev expansion — Structure factor — Operator — Graph

1. Introduction

In original investigation [1], Hosoya and Randić obtained the closed forms of the Chebyshev expansion for an arbitrary star graph and a bicentric tree graph in terms of the "structure factor" expressed as the linear combination of the "step-down operator". In the same article the two authors proposed two conjectures.

In this paper we discuss the properties of "structure factor" and given the rigorous proof of the two conjectures.

2. Properties of "structure factor"

Denote the characteristic polynomial of a path graph having n vertices (i.e. a graph composed of n linearly connected vertices) by $S_n(x)$. [1-4]

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

So called "step down operator" $\mathscr{d}$ is defined as follows[1]

$$\mathscr{d}S_n=S_{n-1} \qquad (n\geq 1), \tag{2}$$

or more generally

$$d^k S_n = S_{n-k} \qquad (n \geq k)\,. \tag{3}$$

It is well known [1, 4, 5] that

$$S_k \cdot S_j = S_{k+j} + S_{k+j-2} + S_{k+j-4} + \cdots + S_{k-j} \qquad (k \geq j \geq 0). \tag{4}$$

By substituting (3) into (4),

$$S_k \cdot S_j = (1 + d^2 + d^4 + \cdots + d^{2j}) S_{k+j} \qquad (k \geq j \geq 1). \tag{5}$$

Let

$$\mathscr{D}_j = d^2 + d^4 + \cdots + d^{2j} \qquad (j \geq 1;\ \mathscr{D}_0 = 0). \tag{6}$$

Thus,

$$S_k \cdot S_j = (1 + \mathscr{D}_j) S_{k+j} \qquad (k \geq j \geq 0). \tag{7}$$

The Chebyshev expansion of the characteristic polynomial of a graph G with n vertices is written as follows [1, 5-8]

$$P_G(x) = \sum_{k=0}^{n} C_k S_{n-k} = S_n + \sum_{k=1}^{n} C_k S_{n-k}. \tag{8}$$

The following recurrence formula is useful

$$P_G(x) = P_{G-L}(x) - P_{G \ominus L}(x), \qquad [6, 7, 9, 10]. \tag{9}$$

Where the meaning of the notations is clear from Fig. 1, in which if the pivot edge L is deleted, the original graph becomes disconnected.

Now we define a proper operator of the form

$$g = \sum_{k=0}^{m} C_k d^k. \tag{10}$$

It is called 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 sufficient length.

Thus, from (8)

$$G_n = g S_n (m \geq n), \tag{11}$$

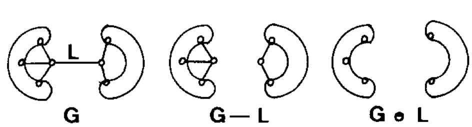

Fig. 1. Illustration of formula (9)

where G_n represents the characteristic polynomial of graph G_n belonging to $\{G_n\}$ (the same notation cannot cause any confusion). Obviously, the "structure factors" obey the associative law, the commutative law and the distributive law of multiplication and addition; i.e. for "structure factors" f, g and h,

$$f \cdot g = g \cdot f, \qquad f + g = g + f;$$
$$f \cdot g \cdot h = (f \cdot g) \cdot h = f \cdot (g \cdot h),$$
$$f + g + h = (f + g) + h = f + (g + h);$$
$$f \cdot (g + h) = f \cdot g + f \cdot h \quad \text{and so on.}$$

The following is a theorem about the properties of "structure factor". This theorem will play an important role in this paper.

Theorem 1. *For a "structure factor" g (see (10)), if $f - m \geq j$ then*

$$(gS_f) \cdot S_j = g(S_f \cdot S_j). \tag{12}$$

Proof.

$$\begin{aligned}(gS_f) \cdot S_j &= \left(\sum_{k=0}^{m} C_k d^k S_f\right) \cdot S_j \\ &= \sum_{k=0}^{m} C_k S_{f-k} \cdot S_j && \text{(from Eq. (3))} \\ &= \sum_{k=0}^{m} C_k (1 + \mathscr{D}_j) \cdot S_{f-k+j} && \text{(from Eq. (7))} \\ &= \sum_{k=0}^{m} C_k (1 + \mathscr{D}_j) d^k S_{f+j} && \text{(from Eq. (3))} \\ &= \left(\sum_{k=0}^{m} C_k d^k\right)((1 + \mathscr{D}_j) S_{f+j}) \\ &= g(S_f \cdot S_j) && \text{(from Eq. (7))} \quad \text{(Q.E.D.).}\end{aligned}$$

3. Proof of Hosoya–Randić conjectures

Let us rewrite Hosoya–Randić conjectures as Theorems 2 and 3.

Theorem 2. *The structure factor for the following star graph G_n with a sufficient length of the tail (Fig. 2) is given by*

$$g = 1 - \sum_{i=2}^{f} (i-1) \cdot \left(\sum_{\substack{k_{t_1} \leq k_{t_2} \leq \cdots \leq k_{t_i} \\ 1 \leq t_1, \ldots, t_i \leq f}} \mathscr{D}_{k_{t_1}} \cdot \mathscr{D}_{k_{t_2}} \cdot \cdots \cdot \mathscr{D}_{k_{t_i}} \right). \tag{13}$$

Proof. For the convenience of writing, we define an operator function as follows,

$$\mathscr{D}(i, f) = \sum_{\substack{k_{t_1} \leq k_{t_2} \leq \cdots \leq k_{t_i} \\ 1 \leq t_1, \ldots, t_i \leq f}} \mathscr{D}_{k_{t_1}} \cdot \mathscr{D}_{k_{t_2}} \cdot \cdots \cdot \mathscr{D}_{k_{t_i}}. \tag{14}$$

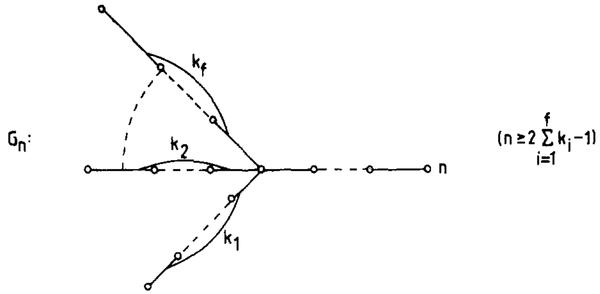

Fig. 2. Star graph

Thus Eq. (13) becomes

$$\mathcal{g} = 1 - \sum_{i=2}^{f} (i-1)\mathcal{D}(i, f). \tag{15}$$

Let us use the inductive method to prove Theorem 2.

For $f = 2$, $k_f = k_2$, choose the line connecting the branch point and the fth branch as the pivot line. According to eq. (9), we have

$$\begin{aligned} G_n &= S_{n-k_2} \cdot S_{k_2} - S_{n-k_1-k_2-1} \cdot S_{k_1} \cdot S_{k_2-1} \\ &= (1+\mathcal{D}_{k_2}) \cdot S_n - [(1+\mathcal{D}_{k_1})S_{n-k_2-1}]S_{k_2-1} \quad \text{(from Eq. (7))} \\ &= (1+\mathcal{D}_{k_2}) \cdot S_n - (1+\mathcal{D}_{k_1})(1+\mathcal{D}_{k_2-1})d^2 S_n \\ &= (1+\mathcal{D}_{k_2}) \cdot S_n - (1+\mathcal{D}_{k_1})\mathcal{D}_{k_2} S_n \\ &= (1-\mathcal{D}_{k_1}\mathcal{D}_{k_2})S_n \\ &= \left[1 - \sum_{i=2}^{f} (i-1)\mathcal{D}(i, f)\right] S_n \qquad (f = 2). \end{aligned}$$

So for $f = 2$, (13) holds.

Then hypothesize for $f = e$, (13) holds. i.e. for a star graph G_n with $e + 1$ branches, the structure factor is

$$\mathcal{g}_e = 1 - \sum_{i=2}^{e} (i-1)\mathcal{D}(i, f). \tag{16}$$

For $f = e + 1$, take the line connecting the branch point and the fth ($f = e + 1$) branch as the pivot line. According to Eq. (9), we have

$$G_n = (\mathcal{g}_e S_{n-k_{e+1}}) \cdot S_{k_{e+1}} - S_{n-k_1-k_2-\cdots-k_e-k_{e+1}-1} \cdot S_{k_1} \cdot S_{k_2} \cdots S_{k_e} \cdot S_{k_{e+1}-1}. \tag{17}$$

From Theorem 1 and Eq. (7),

$$G_n = (\mathcal{g}_e(1+\mathcal{D}_{k_{e+1}}) - (1+\mathcal{D}_{k_1})(1+\mathcal{D}_{k_2}) \cdots (1+\mathcal{D}_{k_e})\mathcal{D}_{k_{e+1}})S_n.$$

Thus

$$\begin{aligned}
\mathscr{g}_{e+1} &= \mathscr{g}_e(1+\mathscr{D}_{k_{e+1}}) - (1+\mathscr{D}_{k_1})(1+\mathscr{D}_{k_2})\cdots(1+\mathscr{D}_{k_e})\mathscr{D}_{k_{e+1}} \\
&= \left[1-\sum_{i=2}^{e}(i-1)\mathscr{D}(i,e)\right](1+\mathscr{D}_{k_{e+1}}) - (1+\mathscr{D}_{k_1})(1+\mathscr{D}_{k_2})\cdots(1+\mathscr{D}_{k_e})\mathscr{D}_{k_{e+1}} \\
&= \left[1-\sum_{i=2}^{e}(i-1)\mathscr{D}(i,e) - \mathscr{D}_{k_{e+1}}\cdot\sum_{i=2}^{e}(i-1)\mathscr{D}(i,e)+\mathscr{D}_{k_{e+1}}\right] \\
&\quad -\left[\mathscr{D}_{k_{e+1}}+\mathscr{D}_{k_{e+1}}\cdot\sum_{i=2}^{e}\mathscr{D}(i,e)+\mathscr{D}_{k_{e+1}}\cdot\sum_{i=1}^{e}\mathscr{D}_{k_i}\right] \\
&= 1-\sum_{i=2}^{e}(i-1)\mathscr{D}(i,e)-\mathscr{D}_{k_{e+1}}\cdot\sum_{i=2}^{e} i\cdot\mathscr{D}(i,e)-\mathscr{D}_{k_{e+1}}\cdot\sum_{i=1}^{e}\mathscr{D}_{k_i} \\
&= 1-\sum_{i=3}^{e+1}(i-1)\mathscr{D}(i,e+1)-D(2,e)-\mathscr{D}_{k_{e+1}}\cdot\sum_{i=1}^{e}\mathscr{D}_{k_i} \\
&= 1-\sum_{i=3}^{e+1}(i-1)\mathscr{D}(i,e+1)-\mathscr{D}(2,e+1) \\
&= 1-\sum_{i=2}^{e+1}(i-1)\mathscr{D}(i,e+1). \qquad (18)
\end{aligned}$$

For $f=e+1$, (13) still holds. Theorem 2 has been proved rigorously.

Theorem 3. *For a graph G_n with two branch points and a sufficiently long tail, as shown in Fig.* 3, *the structure factor is given by*

$$\mathscr{g}=(1-\mathscr{D}_i\mathscr{D}_m)(1-\mathscr{D}_j\mathscr{D}_k)-d^{2h}\mathscr{D}_k\mathscr{D}_m(1+\mathscr{D}_j)^2 \qquad (19)$$

$$=1-(\mathscr{D}_i\mathscr{D}_m+\mathscr{D}_j\mathscr{D}_k+d^{2h}\mathscr{D}_k\mathscr{D}_m)-2d^{2h}\mathscr{D}_j\mathscr{D}_k\mathscr{D}_m+\mathscr{D}_j\mathscr{D}_k\mathscr{D}_h\mathscr{D}_m. \qquad (20)$$

Proof. Take the line connecting the branch point, which is farther away from the tail n, and one of its branches (the branch k) as the pivot line. Using Eq. (9) and Theorem 2 ($f=2$), we have

$$G_n=[(1-\mathscr{D}_i\mathscr{D}_m)S_{n-k}]S_k-[(1-\mathscr{D}_m\mathscr{D}_{h-1})S_{n-k-j-1}]S_j\cdot S_{k-1}.$$

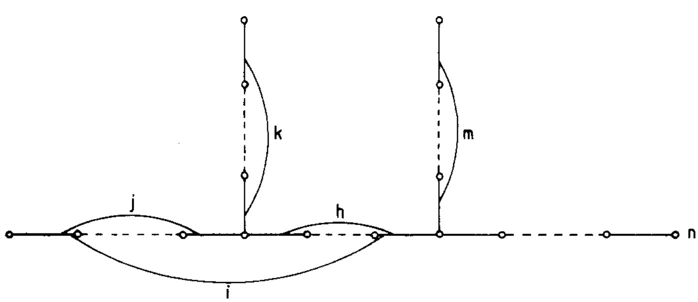

Fig. 3. Bicentric tree graph

From Theorem 1,

$$G_n = [(1-\mathscr{D}_i\mathscr{D}_m)(1+\mathscr{D}_k)-(1-\mathscr{D}_m\mathscr{D}_{h-1})(1+\mathscr{D}_j)\mathscr{D}_k]\,S_n.$$

Therefore,

$$g = (1-\mathscr{D}_i\mathscr{D}_m)(1+\mathscr{D}_k)-(1-\mathscr{D}_m\mathscr{D}_{h-1})(1+\mathscr{D}_j)\mathscr{D}_k. \tag{21}$$

By considering

$$\mathscr{D}_{h-1} = d^2+d^4+\cdots+d^{2h-2} = (d^2+d^4+\cdots+d^{2h})-d^{2h} = \mathscr{D}_h - d^{2h}, \tag{22}$$

$$\begin{aligned} g &= 1-\mathscr{D}_i\mathscr{D}_m-\mathscr{D}_m\mathscr{D}_i\mathscr{D}_k-\mathscr{D}_j\mathscr{D}_k-d^{2h}\mathscr{D}_k\mathscr{D}_m+\mathscr{D}_m\mathscr{D}_h\mathscr{D}_k \\ &\quad +\mathscr{D}_j\mathscr{D}_k\mathscr{D}_h\mathscr{D}_m-d^{2h}\mathscr{D}_j\mathscr{D}_k\mathscr{D}_m-\mathscr{D}_k+\mathscr{D}_k \\ &= -\mathscr{D}_m\mathscr{D}_i\mathscr{D}_k+\mathscr{D}_m\mathscr{D}_h\mathscr{D}_k-d^{2h}\mathscr{D}_m\mathscr{D}_j\mathscr{D}_k+1 \\ &\quad -(\mathscr{D}_i\mathscr{D}_m+\mathscr{D}_j\mathscr{D}_k+d^{2h}\mathscr{D}_k\mathscr{D}_m)+\mathscr{D}_j\mathscr{D}_k\mathscr{D}_h\mathscr{D}_m. \end{aligned} \tag{23}$$

Then by considering

$$\begin{aligned} \mathscr{D}_i &= d^2+d^4+\cdots+d^{2h}+d^{2h+2}+\cdots+d^{2h+2j} \\ &= \mathscr{D}_h+d^{2h}\mathscr{D}_j, \end{aligned} \tag{24}$$

and substituting (24) into the first term of (23), we get

$$g = 1-(\mathscr{D}_i\mathscr{D}_m+\mathscr{D}_j\mathscr{D}_k+d^{2h}\mathscr{D}_k\mathscr{D}_m)-2d^{2h}\mathscr{D}_m\mathscr{D}_j\mathscr{D}_k+\mathscr{D}_j\mathscr{D}_k\mathscr{D}_h\mathscr{D}_m, \tag{25}$$

which is nothing else but Eq. (20).

From Eq. (20), we have

$$\begin{aligned} g &= (1-\mathscr{D}_i\mathscr{D}_m)(1-\mathscr{D}_j\mathscr{D}_k)-d^{2h}\mathscr{D}_k\mathscr{D}_m(1+2\mathscr{D}_j)+\mathscr{D}_j\mathscr{D}_k\mathscr{D}_h\mathscr{D}_m-\mathscr{D}_i\mathscr{D}_j\mathscr{D}_k\mathscr{D}_m \\ &= (1-\mathscr{D}_i\mathscr{D}_m)(1-\mathscr{D}_j\mathscr{D}_k)-d^{2h}\mathscr{D}_k\mathscr{D}_m(1+2\mathscr{D}_j)-\mathscr{D}_j\mathscr{D}_k\mathscr{D}_m(\mathscr{D}_i-\mathscr{D}_h) \\ &= (1-\mathscr{D}_i\mathscr{D}_m)(1-\mathscr{D}_j\mathscr{D}_k)-d^{2h}\mathscr{D}_k\mathscr{D}_m(1+2\mathscr{D}_j) \\ &\quad -\mathscr{D}_j\mathscr{D}_k\mathscr{D}_m(\mathscr{D}_h+d^{2h}\mathscr{D}_j-\mathscr{D}_h) \quad \text{(from Eq. (24))} \\ &= (1-\mathscr{D}_i\mathscr{D}_m)(1-\mathscr{D}_j\mathscr{D}_k)-d^{2h}\mathscr{D}_k\mathscr{D}_m(1+2\mathscr{D}_j+\mathscr{D}_j^2) \\ &= (1-\mathscr{D}_i\mathscr{D}_m)(1-\mathscr{D}_j\mathscr{D}_k)-d^{2h}\mathscr{D}_k\mathscr{D}_m(1+\mathscr{D}_j)^2 \end{aligned}$$

which is nothing else but Eq. (19).

As seen above, Theorem 1 is very useful for determining the structure factors of many series of characteristic graphs by recurrence method. Particularly, by combining it with many efficient techniques for expanding and solving the characteristic polynomials of complex graphs, such as the partition technique [11, 12], the pruning technique [13, 14], the block-diagonalization method and so on, [4, 6, 7, 9–16] it can be used in more extensive field.

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