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Review Article

Equitable partitions and spectra of symmetric trees: Revisiting Heilbronner's composition principle

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Abstract

The notion of equitable partitions, first defined by Horst Sachs, embodies a notable procedure in spectral graph theory, which is far from being conveniently explored in the literature. With equitable partitions, we can deduce significant spectral properties of a graph. For trees with a high level of symmetry, we can combine this technique with the "composition principle" (developed by Edgar Heilbronner more than seven decades ago) and fully determine the entire spectrum. This is a partially survey note where we provide several descriptive examples of this combination. We show that some recent results on the factorization of the characteristic polynomials of symmetric trees can be derived by merging both methods.

Keywords: equitable partitions; symmetric graphs; eigenvalues.

2020 Mathematics Subject Classification: 15A18, 15A03, 05C50.

1. Introduction

For a given simple graph G, we say that $V(G) = V_1 \sqcup V_2 \sqcup \cdots \sqcup V_k$ is an *equitable partition* if every vertex in V_i has the same number of neighbors in V_j, for any $i, j \in \{1, 2, \ldots, k\}$. Corresponding to G, we consider the weighted digraph with vertex set $\{V_1, V_2, \ldots, V_k\}$, where the weight of the arc (i, j) is the number b_{ij} of those neighbors that each vertex of V_i has in V_j. This digraph is called a *divisor graph* of G (divisor of G, in short), and its $k \times k$ (weighted) adjacency matrix is called a *divisor matrix*. For example, if we consider the tree depicted in Figure 1, then one of its equitable partitions, which we will call *canonical*, is

$$\Pi \;:\; V_1 = \{1\}\,,\; V_2 = \{2, 3\}\,,\; V_3 = \{4, 5, 6, 7, 8, 9\},$$

with the following divisor matrix:

$$D_\Pi = \begin{pmatrix} 0 & 2 & 0 \\ 1 & 0 & 3 \\ 0 & 1 & 0 \end{pmatrix}.$$

Thus, D_Π represents the weighted adjacency matrix of the divisor (which is a directed path) depicted in Figure 2. The rooted tree of Figure 1 is known [9] as a balanced tree since the vertices of the same level have an equal degree.

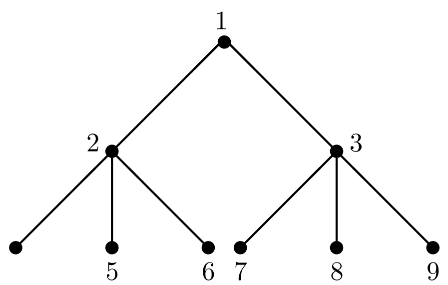

Figure 1: A balanced tree.

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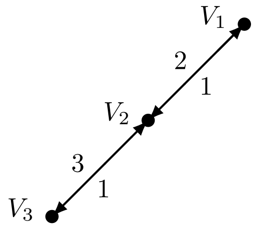

Figure 2: A divisor graph of $T^1_{1,3,2}$.

The notion of a divisor (*Teiler*) of a graph was first introduced in the second half of the 1960s in two seminal papers [29, 30] by the German mathematician and recipient of the 2000 Euler Medal, Horst Sachs (cf. [4]). Among the many remarkable properties, we know that the characteristic polynomial of a divisor divides the characteristic polynomial of the graph [6, Theorem 3.9.5]. This means, for example, that an eigenvalue of a divisor matrix is also an eigenvalue of the original graph [6, Theorem 3.9.5]. Of course, the multiplicity of any eigenvalue of the divisor is less than or equal to the multiplicity as eigenvalue of the graph. Furthermore, the index (i.e., the largest eigenvalue) of a graph is an eigenvalue of any of its divisors (cf. [6, Corollary 3.9.11]).

In [5, p.130], it is defined a *symmetric tree* $T^q_{r,m}$ *of degree* r, with $q = 1, 2$, $r \geqslant 3$, and $m \geqslant 0$, as a tree such that

(i) each vertex has either degree 1 or degree r;

(ii) there is a *central element* c which is a vertex if $q = 1$, or an edge if $q = 2$;

(iii) the distance between c and each pendent vertex equals m.

A symmetric tree of the first type is also known in [9] as dendrimer and in [10] is denoted by $\hat{X}^r_{m-1}$.

The symmetric trees were studied in 1973 by Finck and Sachs [12, p.84]. They considered as examples of type one: $T^1_{3,1}$, which is a star on 4 vertices, and $T^1_{4,2}$, which consists of four copies of $T^1_{3,1}$ conveniently joined to a center; and of type two: $T^2_{5,2}$ and $T^2_{3,1}$. In [5, Figure 4.8], we can find $T^1_{4,2}$ and $T^2_{3,2}$ as examples (see Figure 3).

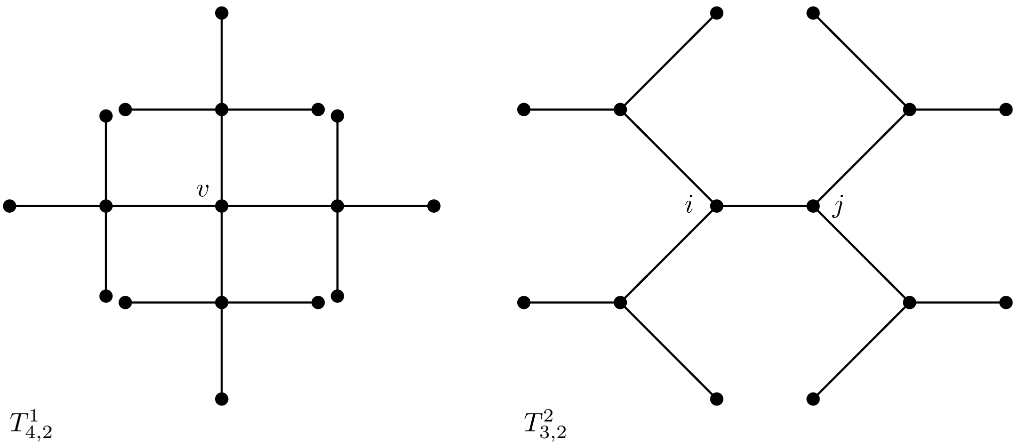

Figure 3: Examples of symmetric trees.

In the case of $T^1_{4,2}$, the central element is the root vertex v while for $T^2_{3,2}$ is the bridge (i, j). Notice, that $T^2_{3,2}$ consists of 4 copies of a star of order 3 where a pair of centers is joined to a vertex of the central edge while the other pair of centers is joined to the other vertex of the edge. We observe that the central edge provides two types of symmetry in the tree.

This type of symmetric structures was pioneered by Dénes Kőnig in his comprehensive treatise [20] in a more general setting (see, for example, Figure 68-71 in Kőnig's masterpiece).

Notwithstanding, the aim of Finck and Sachs was to study the spectral properties of regular graphs of degree r covered in a certain way by $T^2_{r,m}$. They proved that such graphs always contain as eigenvalues

$$2\sqrt{r-1}\cos\frac{k\pi}{m+1}\,, \quad \text{for } k = 1, 2, \ldots, m.$$

These eigenvalues correspond to those of the tridiagonal matrix

$$D = \begin{pmatrix} 0 & r-1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & r-1 \\ & & 1 & 0 \end{pmatrix}_{m\times m}.$$

However, for symmetric trees and, more generally, for generalized Bethe trees, (i.e., rooted trees with a given number of levels in which vertices at the same level have the same degree), we can fully determine the spectrum based on the spectra of the divisor of the canonical equitable partition of each branch. For that purpose, we will have to go back to the mid-1950s and to two groundbreaking papers of the Swiss chemist Edgar Heilbronner. Both works remain largely ignored in the mathematical community. According to John and Sachs [18], in 1953,

> *E. Heilbronner [16] invented the "composition principle"; he was the first to utilize the symmetries of a hydrocarbon in order to simplify the calculation of its characteristic polynomial by means of some folding operations [15].*

Many other authors then follow more or less independently similar procedures. Perhaps the other notorious factorization was due to Collatz and Sinogowitz in 1957 with paper [3].

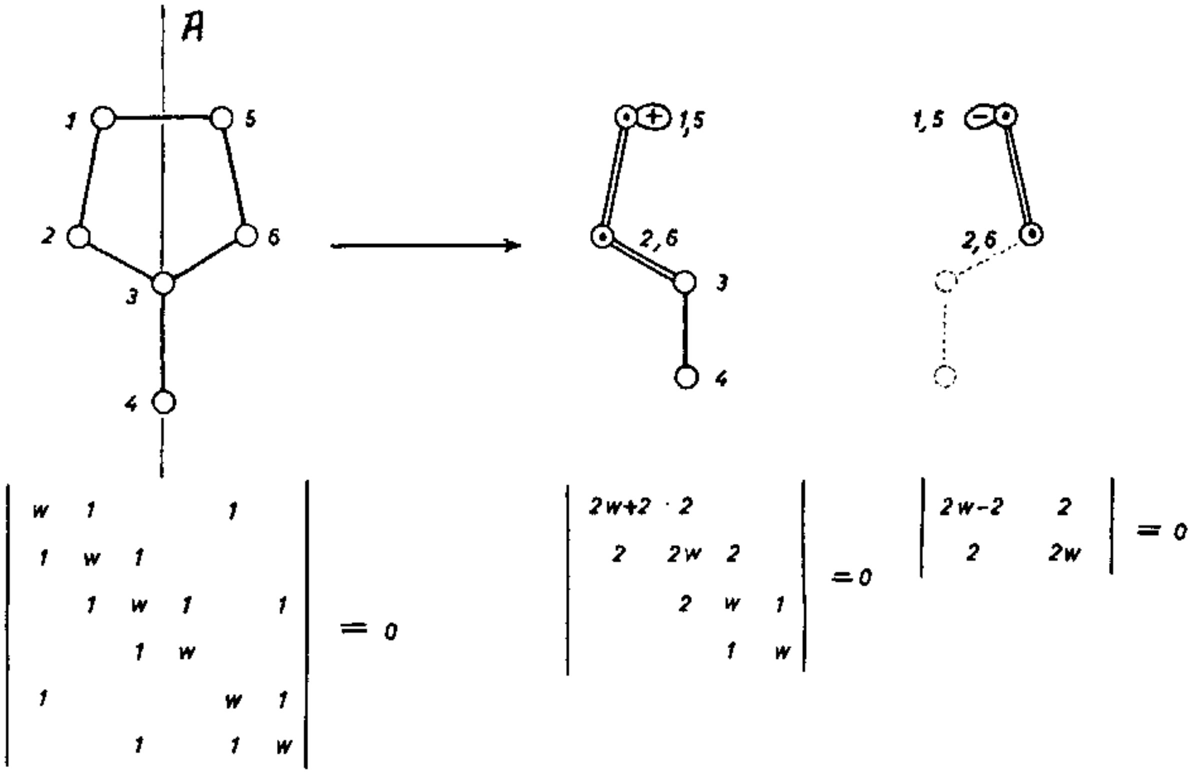

Figure 4: Heilbronner's original example of "positive folding" [15].

We believe that the most likely reason for the widespread lack of awareness of Heilbronner's work in mathematics (and to a lesser extent in chemistry) today is probably because his work was written in German. On the other hand, his results always had a strong emphasis on chemistry, being published and studied mainly in this scientific field.

Before we proceed, we remark that we call all the previous trees symmetric without distinction.

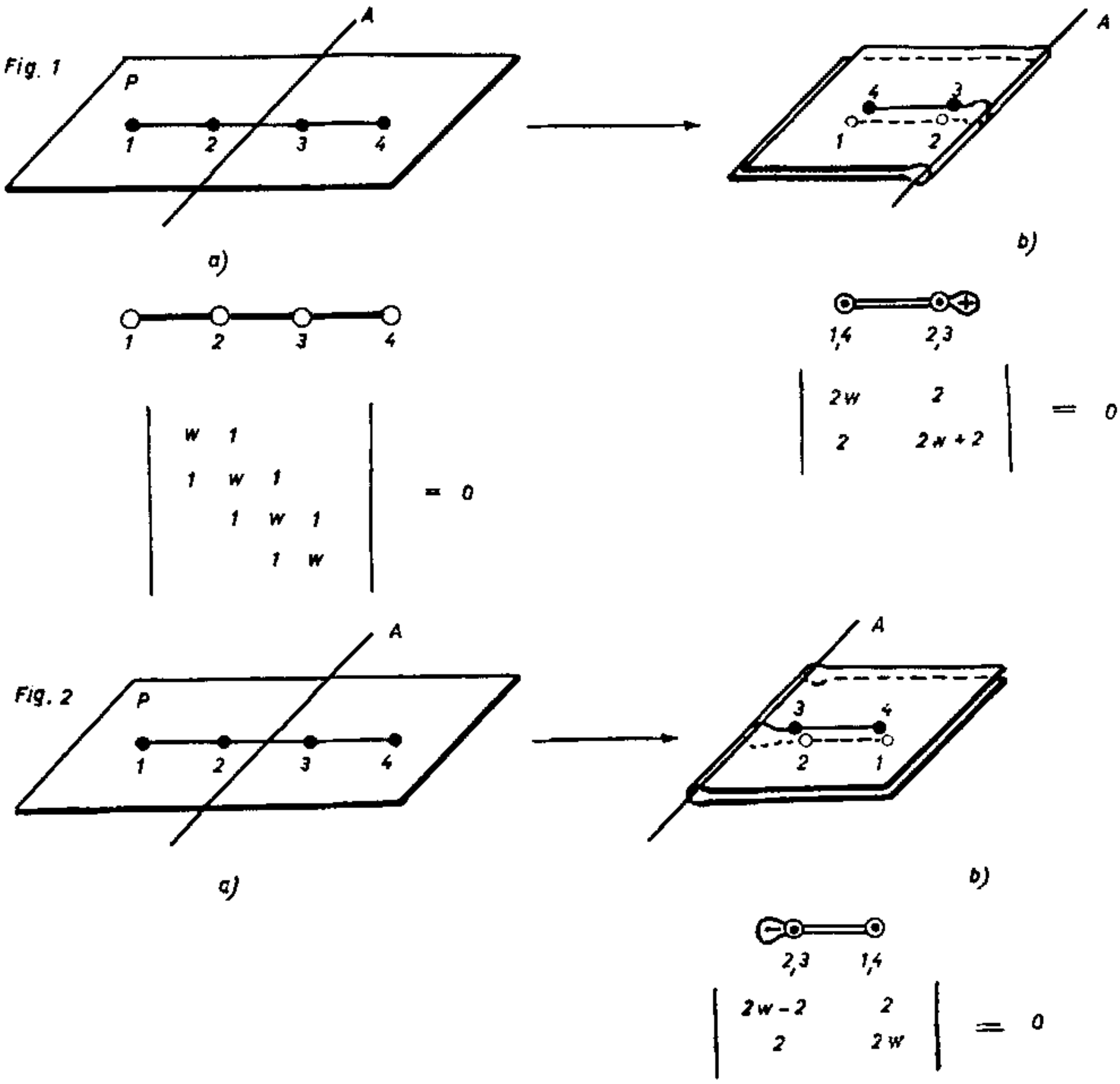

Figure 5: Heilbronner's example of "positive" and "negative foldings" [15].

Heilbronner's method was replicated, explored, extended, and refined mainly in problems associated to chemistry throughout the years. In 1974, McClelland provides the first mathematical contextualization of this method. Indeed, the note [24] is exclusively dedicated to the mathematization of Heilbronner's method. In fact, it contains a single bibliographical reference: Heilbronner's article. Since then Heilbronner's method has become known to many as the *McClelland Method* or *McClelland's rules on graph splitting*. Živković, Trinajstić, and Randić in [34] considered general symmetric graphs where the spectrum is fully determined by the spectra of their "constituting fragments". In [19], Kassman extends the technique of Heilbronner to the determination of the eigenvectors. Sorokin [32] generalizes the construction of the characteristic polynomial of molecular graphs with a symmetric plane. In 1979, D'Amato [7, 8] studied the spectrum for graphs with multifold symmetry (see also [11, 22, 23, 25] for other instances). Noteworthy is the work of Shen [31] where this method is extended to general weighted multi-layered graphs. For multi-symmetries, the reader is referred to the recent paper [21]. Although there is a plethora of articles with particular families of graphs, we believe these are the key milestones.

Inspired by [24, 32, 34], in a somewhat modern language, we describe next with examples the two major folding techniques proposed by Heilbronner (see Figure 4). We will start with the example of the tree $T^1_{1,2,3}$, depicted in Figure 6. Soon we will understand the reason for adopting this notation.

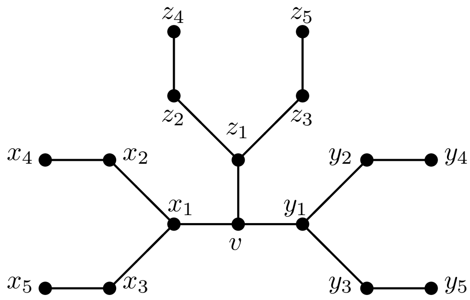

Figure 6: The tree $T^1_{1,2,3}$.

According to [15, Theorem, p.916], the "positive folding" is preserved and in the case of the above tree, it will lead to the characteristic polynomial of the divisor matrix

$$D_{\Pi_3} = \begin{pmatrix} 0 & 3 & & \\ 1 & 0 & 2 & \\ & 1 & 0 & 1 \\ & & 1 & 0 \end{pmatrix}$$

associated to the (canonical) equitable partition

$$\begin{aligned} \Pi_3 \quad : \quad & V_1 = \{v\}\,,\ V_2 = \{x_1, y_1, z_1\}\,, \\ & V_3 = \{x_2, x_3, y_2, y_3, z_2, z_3\}\,,\ V_4 = \{x_4, x_5, y_4, y_5, z_4, z_5\}\,, \end{aligned}$$

whereas the "negative folding" *disappears* giving rise the characteristic polynomial of the subgraph of Figure 7

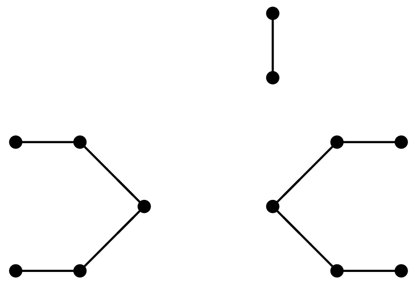

Figure 7: A subgraph of $T^1_{1,2,3}$.

With a straightforward inductive argument, we may conclude that the characteristic polynomial can be factorized as

$$\phi_{\Pi_3}(x)\,\phi_{\Pi_2}(x)^2\,\phi_{\Pi_1}(x)^3\,, \tag{1}$$

where $\phi_{\Pi_2}(x)$ and $\phi_{\Pi_1}(x)$ are the characteristic polynomials of

$$D_{\Pi_2} = \begin{pmatrix} 0 & 2 & \\ 1 & 0 & 1 \\ & 1 & 0 \end{pmatrix} \quad \text{and} \quad D_{\Pi_1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,,$$

respectively.

As always in this area, the methods are quite graphical. For example, the factorization (1) is described in Figure 8.

A different graphic approach can be found, for example in [21].

In general, if we have a rooted tree where at the level $k(>0)$ the vertices have the same *down* degree r_k (i.e., with degree r_k+1), which we denote by $T^1_{r_1,\ldots,r_m}$, then its characteristic polynomial is given by

$$\prod_{\ell=1}^{m} \phi_{\Pi_\ell}(x)^{(r_{\ell+1}-1)r_{\ell+2}\cdots r_m}\,, \tag{2}$$

where ϕ_{Π_ℓ} is the characteristic polynomial of

$$D_{\Pi_\ell} = \begin{pmatrix} 0 & r_\ell & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & r_1 \\ & & 1 & 0 \end{pmatrix}\,, \quad \text{for } \ell = 1, \ldots, m.$$

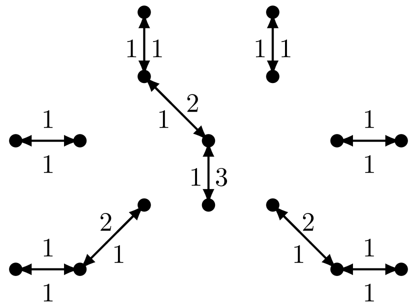

Figure 8: Divisor graph of $T^1_{1,2,3}$.

Notice that Π_ℓ is precisely the canonical equitable participation of the symmetric branch $T^1_{r_\ell,\dots,r_m}$. The vacuous product in (2) should be read as 1 and, for $\ell = m-1$, the power of $\phi_{\Pi_{m-1}}(x)$ is $r_m - 1$.

In case we join the centers of two trees $T^1_{r_1,\dots,r_m}$ by an edge, we get the tree which we will designate by $T^2_{r_1,\dots,r_m}$, from which we obtain a "positive folding" and a "negative folding" along a straight line perpendicular to the bridge [15, p.915]. Take as an example two copies of the tree $T^1_{1,2,3}$ where we connect both roots by an edge. Then one of the factors of the characteristic polynomial of given tree is the characteristic polynomial of the canonical matrix divisor $T^2_{1,2,3}$,

$$D^+_{\Pi_3} = \begin{pmatrix} 1 & 3 & & \\ 1 & 0 & 2 & \\ & 1 & 0 & 1 \\ & & 1 & 0 \end{pmatrix}$$

which is associated to the canonical equitable partition of $T^1_{2,3,3}$. Related to the "negative folding", we have another factor which is the characteristic polynomial of the matrix

$$D^-_{\Pi_3} = \begin{pmatrix} -1 & 3 & & \\ 1 & 0 & 2 & \\ & 1 & 0 & 1 \\ & & 1 & 0 \end{pmatrix}.$$

The remaining factors are $\phi_{\Pi_2}(x)$ and $\phi_{\Pi_1}(x)$. Thus, applying the previous method to the disconnected branches, the characteristic polynomial of $T^2_{1,2,3}$ is

$$\phi^+_{\Pi_3}(x)\,\phi^-_{\Pi_3}(x)\,(\phi_{\Pi_2}(x)^2\,\phi_{\Pi_1}(x)^3)^2\,.$$

From here, we readily extend the factorization formula of the characteristic polynomial for any tree $T^2_{r_1,\dots,r_m}$:

$$\phi^+_{\Pi_m}(x)\,\phi^-_{\Pi_m}(x)\prod_{\ell=1}^{m-1}\phi_{\Pi_\ell}(x)^{2(r_{\ell+1}-1)r_{\ell+2}\cdots r_m}\,, \tag{3}$$

where

$$D^\pm_{\Pi_m} = \begin{pmatrix} \pm1 & r_m & & & \\ 1 & 0 & r_{m-1} & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & r_1 \\ & & & 1 & 0 \end{pmatrix}.$$

In the particular cases of the symmetric trees $B^q_{r,m}$ considered by Finck and Sachs [12], for $q=1$, we have $T^1_{r-1,\dots,r-1,r}$, while for $q=2$, we have $T^2_{r-1,\dots,r-1}$, each with m subindexes. Therefore, the characteristic polynomial of $T^1_{r,m}$ can be factorized as

$$\phi_{\Pi_m}(x)\,\phi_{\Pi_{m-1}}(x)^{r-1}\prod_{\ell=1}^{m-2}\phi_{\Pi_\ell}(x)^{(r-2)(r-1)^{m-\ell-2}r}\,, \tag{4}$$

while for $T^2_{r,m}$ we get

$$\phi^+_{\Pi_m}(x)\,\phi^-_{\Pi_m}(x)\prod_{\ell=1}^{m-1}\phi_{\Pi_\ell}(x)^{2(r-2)(r-1)^{m-\ell-1}}\,. \tag{5}$$

Another trivial application is when we apply Heilbronner's procedures to a path. For a path of odd order $2t+1$, the characteristic polynomial can be factorized as a product of the characteristic polynomials of the divisor matrices

$$\begin{pmatrix} 0 & 2 & & & \\ 1 & 0 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 0 \end{pmatrix}_{(t+1)\times(t+1)} \quad \text{and} \quad \begin{pmatrix} 0 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{pmatrix}_{t\times t}.$$

Otherwise, the order is $2t$, which means that the factorization corresponds to the matrices

$$\begin{pmatrix} 1 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 0 \end{pmatrix}_{t\times t} \quad \text{and} \quad \begin{pmatrix} -1 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 0 \end{pmatrix}_{t\times t},$$

representing the positive and negative foldings about the central edge.

We will discuss in the next section, how these factorizations can be found in the recent literature.

It is worth mentioning that Heilbronner explained in [15] how to combine the two folding strategies for graphs (not necessarily acyclic) with several symmetries, as we see in Figures 9 and 10. We believe that this is still far from being well explored in modern literature. We leave this discussion for further investigation.

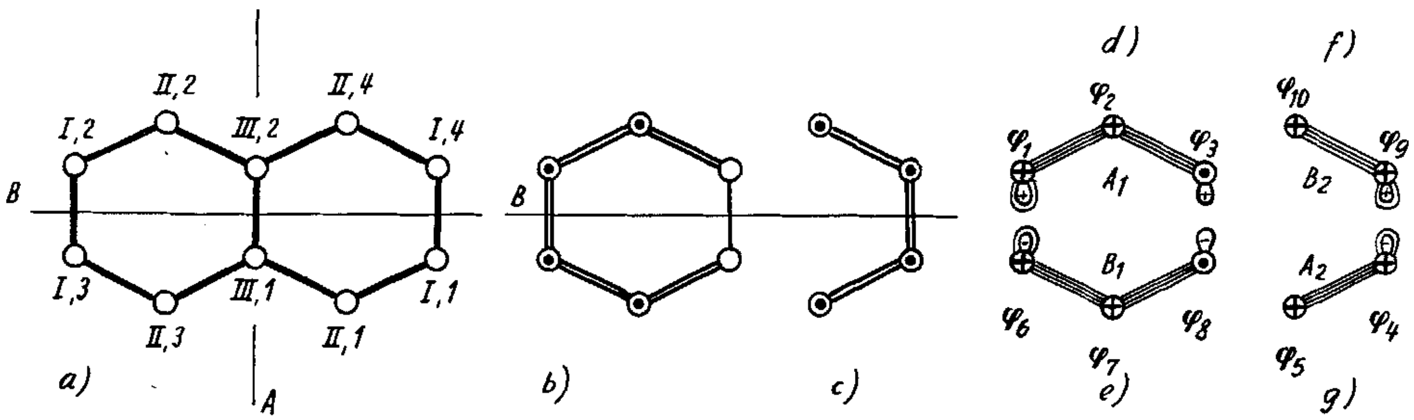

Figure 9: An example proposed by Heilbronner of a sequence of symmetries and its foldings [15].

Darstellung A_1 — Darstellung B_1 — Darstellung B_2 — Darstellung A_2

$$\left\| \begin{matrix} 4w+4 & 4 & \\ 4 & 4w & 4 \\ & 4 & 2w+2 \end{matrix} \right\| = \left\| \begin{matrix} 4w-4 & 4 & \\ 4 & 4w & 4 \\ & 4 & 2w-2 \end{matrix} \right\| = \left\| \begin{matrix} 4w+4 & 4 \\ 4 & 4w \end{matrix} \right\| = \left\| \begin{matrix} 4w-4 & 4 \\ 4 & 4w \end{matrix} \right\| = 0.$$

Figure 10: The factors [15].

2. Comments on some recent results

In the last two decades, symmetric trees and their extensions have been independently rediscovered. For example, in 2005, Rojo and Soto [27], considered the family $\mathcal{T}$ of unweighted rooted trees of k levels such that in each level the vertices have equal degree. Indeed, they were considering the matrices of type 1 analyzed in [12]. The factorization for the characteristic polynomial is provided in (2).

In [26], it is considered the particular case of the Bethe trees $B_{d,k}$ where the root vertex has degree d and in the remaining levels (excluding, of course, the ground level) is $d+1$. This gives rise to tridiagonal Toeplitz matrices for the divisor matrices. Notice that [27, Corollary 8] says that the index of a graph coincides with the largest eigenvalue of a particular divisor matrix. This result, as we pointed out, it is indeed true for any divisor matrix. Moreover, in [26, Theorem 7], besides the inaccuracy with the range of the indexes j and l, the multiplicities can in fact be higher than claimed.

In [10], the k-ary rooted tree of depth r, X_r^k, is precisely the symmetric tree $T^1_{k,\dots,k}$, while $\hat{X}_r^k$ is $T^2_{k-1,\dots,k-1,k}$, where the sub-indexes appear $(r+1)$-times. Here, we would like to make some comments. The polynomial $Q_n^k(x)$ defined in [10, (3.1)] is $\phi^k_{n+1}(x)$ as we can find earlier in this note. Theorem 5 is then a consequence of (2). On the other hand, in Section 4, the authors discussed the trees $X_{2n}^{(\alpha,\beta)}$ with the so-called 2-periodic branching and provided some considerations for longer periods. In this case, the divisor matrices are 2-Toeplitz matrices, which are well-known in the literature. The general study of the spectra of these matrices goes back more than five decades with the work by Pál Rózsa [28]. We can also find them, for example, in the context of the orthogonal polynomials [13, 14]. For a more historical bibliography, the reader is referred to [2].

Recently, in [1], it was studied the spectrum of the p-sun, a tree with $2p+1$ vertices where p paths of order 2 are attached to a common single vertex, that is, $T^1_{1,p}$ (in the sense of the definition of this note). The authors used a powerful algorithm established in [17], which determines the characteristic polynomial of a general tree. Nevertheless, since a p-sun is the tree $T^1_{1,p}$, its characteristic polynomial follows from (2):

$$p(x) = x(x^2-p-1)(x^2-1)^{p-1},$$

corresponding to the divisor matrices

$$\begin{pmatrix} 0 & p & \\ 1 & 0 & 1 \\ & 1 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Clearly, we can extend this result to any p-sun where each sunray is a path of a fixed length n. Recall that the characteristic polynomial of the tridiagonal matrix

$$\begin{pmatrix} 0 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{pmatrix}_{n\times n}$$

is $U_n(x/2)$, where $U_n(x)$ is the Chebyshev polynomial of the second kind of order n.

For the (p,q)-double sun, i.e., one p-sun and one q-sun with both roots connected by a bridge, we can still use Heilbronner's procedure. Considering the case $p=q$ and each sunray is a path of a fixed length n, the "positive folding" will lead to the characteristic polynomial of the divisor matrix

$$\begin{pmatrix} 1 & p & & & \\ 1 & 0 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 0 \end{pmatrix}_{(n+1)\times(n+1)},$$

while the "negative folding" gives rise to the characteristic polynomial of the tridiagonal matrix

$$\begin{pmatrix} -1 & p & & & \\ 1 & 0 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & 0 \end{pmatrix}_{(n+1)\times(n+1)}.$$

The other factor is $U_n(x/2)$ with multiplicity $2(p-1)$.

In the generalized case of a (p, q)-double sun with distinct numbers of lengths for the sunrays of each branch, say m and n for the p and q-suns, respectively, we have to make a positive folding along the path containing two distinct sunrays and the bridge. The characteristic polynomial will be factorized as

$$\phi_\Pi(x)\,(U_m(x/2))^{p-1}\,(U_n(x/2))^{q-1}\,,$$

where $\phi_\Pi(x)$ is the characteristic polynomial of the divisor matrix

$$D_\Pi = \left(\begin{array}{ccccc|ccccc} 0 & 1 & & & & & & & & \\ 1 & \ddots & \ddots & & & & & & & \\ & \ddots & \ddots & 1 & & & & & & \\ & & 1 & 0 & 1 & & & & & \\ & & & p & 0 & 1 & & & & \\ \hline & & & & 1 & 0 & q & & & \\ & & & & & 1 & 0 & 1 & & \\ & & & & & & 1 & \ddots & \ddots & \\ & & & & & & & \ddots & \ddots & 1 \\ & & & & & & & & 1 & 0 \end{array}\right),$$

where the first block is of order $m + 1$ and the second of order $n + 1$. Consider, for example, the generalized $(2, 3)$-double sun depicted in Figure 11. Graphically, the factorization can be represented as in Figure 12.

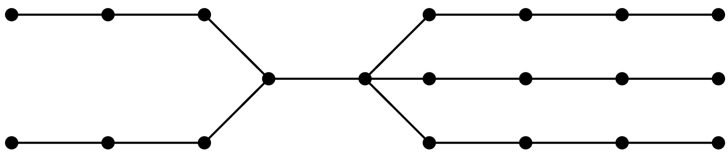

Figure 11: The generalized $(2, 3)$-double sun.

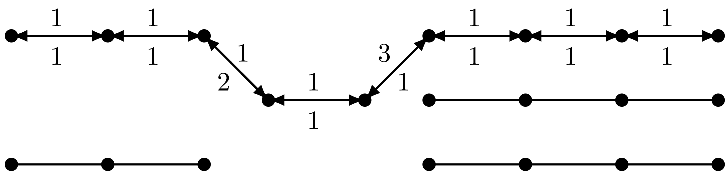

Figure 12: Factorization of the generalized $(2, 3)$-double sun.

In the recent papers [9, 33], the spectral properties of balanced trees and dendrimers were investigated. As we mentioned elsewhere, a balanced tree is a rooted tree $T^1_{r_1,\ldots,r_m}$, while a dendrimer is a symmetric tree in the sense of Finck and Sachs [12], i.e., a rooted tree of the type $T^1_{r-1,\ldots,r-1,r}$. Theorem 3 in [9] is a consequence of the factorization (2). The sequence of the polynomials $Q_n(x)$ corresponds to the the characteristic polynomials ϕ_{Π_ℓ} of the divisor matrices D_{Π_ℓ}. The proof of this theorem relies on the *characteristic matrices* (cf. [6, p.84]) of the (canonical) equitable partitions.

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