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Abstract: In 1971, Graham and Pollack established a relationship between the number of negative eigenvalues of the distance matrix and the addressing problem in data communication systems. They also proved that the determinant of the distance matrix of a tree is function of the number of vertices only. Since then several mathematicians were interested in studying the spectral properties of the distance matrix of a connected graph. Computing the distance characteristic polynomial and its coefficients was the first research subject of interest. Thereafter, the eigenvalues attracted much more attention. In the present paper, we report on the results related to the distance matrix of a graph and its spectral properties.

Key Words: Distance matrix, eigenvalues, largest eigenvalue, characteristic polynomial, graph.

Résumé : En 1971, Graham et Pollack ont établi un lien entre le nombre de valeurs propres negatives de la matrice des distances et le problème d'adressage dans les systèmes de communication de données. Ils ont aussi prouvé que le déterminant de la matrice des distances d'un arbre s'écrit en fonction du nombre de ses sommets uniquement. Depuis, plusieurs mathématiciens se sont intéressés à l'étude des propriétés spectrales de la matrice des distances d'un graphe connexe. Au début, l'intérêt fut porté sur le calcul du polynôme caractéristique et de ses coefficients. Puis, les valeurs propres ont succité beucoup plus d'intérêt. Dans le présent article, nous proposons une vue d'ensemble des résultats sur la matrice des distances et ses propriétés spectrales.

Mots clés : Matrice des distances, valeurs propres, plus grande valeur propre, polynôme caractéristique, graphe.

1 Introduction

There are mainly two versions of the distance matrix of a graph: *graph–theoretical* and *geometric*. For a connected graph, the distance matrix, in the case of graph–theoretical version, is a natural generalization, with more specificity, of the adjacency matrix. The distance between two vertices is defined as the length (number of edges) of a shortest path between them. In the case of the geometric version, we consider points in a plane and the distances correspond to the Euclidean distance. In this case, we speak more about points in a *metric space* than about vertices in a graph. The origins of the distance matrix goes back to the very first paper of Cayley [34] in 1841. However, its study began formally during the 20^{th} century [118, 141]. Graph theory researchers were first interested in the problem of realizability of the distance matrix. Namely, for a given real symmetric $n \times n$–matrix $D = (d_{i,j})$ such that $d_{i,i} = 0$ and $0 \leq d_{i,j} \leq d_{i,k} + d_{k,j}$, $1 \leq i, j, k \leq n$, is there a graph G for which D is the distance matrix. This problem was first posed by Hakimi and Yau [69], and then studied by many mathematicians among which we cite Simões–Pereira [120, 122, 124, 125], Buneman [28], Simões–Pereira and Zamfirescu [126], Varone [137], Boesch [18], Patrinos and Hakimi [107], Bandelt [13], and Nieminen [104]. Dress [52] proved that any shortest path distance matrix can be realized by a minimum weight graph. In the case of trees, efficient algorithms stating how to find this optimal solution have been developed [18, 40, 107, 126]. However, in the case of general graphs, only a few results are known concerning the structure of optimal realizations (see e.g. [53, 72, 80, 89]), and dealing with the problem is much harder. Indeed, although it is well–known that an optimal realization exists [52, 123], Althöfer [1] and Winkler [140] showed that the problem is NP–complete if the distance matrix has integer entries. Actually, many heuristic methods were proposed [53, 72, 104, 120, 121, 126, 136], however, computing optimal realizations of general distance matrices is still difficult.

The second aspect of distance matrix that kept the attention of the mathematicians is the study of its spectral properties. In this case, the focus was more on the graph theoretical version of the matrix. The interest began during the 70's with the appearance of the paper [64] by Graham and Pollack. In that paper the authors established a relationship between the number of negative eigenvalues of the distance matrix and the addressing problem in data communication systems. In the same paper [64], it was proved that the determinant of the distance matrix of a tree is function of the number vertices only. This impressive result made distance matrix spectral properties a research subject of great interest. Graham and Lovász [62] computed the inverse of the distance matrix of a tree. Edelberg, Garey and Graham [55], Graham and Lovász [62], and Hosoya, Murakami and Gotoh [74] studied the characteristic polynomial. Actually, they calculated certain, and in some cases all, the coefficients of the distance characteristic polynomial. Merris [100] provided the first estimation of the distance spectrum of a tree. Many other authors studied the distance spectrum of a graph, we report about their works below. Recently, the maximum or the minimum values of the distance spectral radius of a given class of graphs has been studied extensively.

Several domains of application of the distance matrix, in an implicit or an explicit form, are known: the design of communication networks [56, 64], network flow algorithms [51, 59], graph embedding theory [49, 55, 62, 63, 65] as well as molecular stability [74, 152]. Balaban, Ciubotariu and Medeleanu [9] proposed the use of the distance spectral radius as a molecular descriptor (see also [39, 134]). Gutman and Medeleanu [68] used the distance spectral radius to infer the extent of branching and model boiling points of an alkane (see also [19]). For other applications in chemistry see [73, 101, 113, 114, 115] as well as the books [8, 86, 135], and the references therein. Among other branches of sciences where the notion of distance in graphs (thus the distance matrix in an implicit form), we can cite psychology [41], phylogenetic [48, 92], software compression [93], analysis of Internet infrastructures [35], modeling of traffic [29, 30], and social networks [60, 87, 117, 119, 139].

In the present survey, we focus on the research related to the spectral properties of the distance matrix in its graph–theoretical version. We begin by recalling some definitions.

We consider only simple, finite and connected graphs, *i.e*, graphs on a finite number of vertices without multiple edges or loops and in which any two vertices are linked by a sequence of edges. A graph is (usually) denoted by $G = G(V, E)$, where V is its vertex set and E its edge set. The *order* of G is the number $n = |V|$ of its vertices and its *size* is the number $m = |E|$ of its edges. The *adjacency matrix* of G is a 0–1 $n \times n$–matrix indexed by the vertices of G and defined by $a_{ij} = 1$ if and only if $ij \in E$. For details on the adjacency matrix and its spectrum see the books [26, 42, 43, 44, 133]. The *degree* d_i of the vertex $i \in V$ is the number of vertices adjacent to i, *i.e.*, the sum of the i^{th} row (column) of the adjacency matrix of G. Let Δ and δ denote the maximum and minimum degrees of G, respectively. If $G = (V, E)$ is a graph, $v \in V$ and $e \in E$, then v (resp. e) is a cut vertex (resp. edge) of G if $G - v$ (resp. $G - e$) is disconnected. As usual, we denote by P_n the path, by C_n the cycle, by S_n the star, by $K_{a,n-a}$ the complete bipartite graph and by K_n the complete graph, each on n vertices.

The distance matrix $\mathcal{D}$ of a graph G is the matrix indexed by the vertices of G where $\mathcal{D}_{i,j} = d_{ij} = d(v_i, v_j)$ and $d_{ij} = d(v_i, v_j)$ denotes the distance between the vertices v_i and v_j, *i.e*, the length of a shortest path between v_i and v_j (for properties of distances in graphs see the book by Bukley and Harary [27] and the references therein). The maximum distance between two vertices is called the *diameter* of G and denoted by $D = D(G)$, *i.e.*, $D = D(G) = \max\{d(u, v) \ : \ u, v \in G\}$. The characteristic polynomial of $\mathcal{D}(G)$ is defined by $P_{\mathcal{D}}(t) = P_{\mathcal{D}(G)}(t) = Det\,(tI - \mathcal{D}(G))$, where I is $n \times n$ identity matrix. It is called the *distance characteristic polynomial* of G. Since $\mathcal{D}(G)$ is a real symmetric matrix, all its eigenvalues, called *distance eigenvalues* of G, are real. The spectrum of $\mathcal{D}$ is denoted by $\{\partial_1, \partial_2, \ldots, \partial_n\}$ and indexed such that $\partial_1 \geq \partial_2 \geq \cdots \geq \partial_n$. It is called the *distance spectrum* of the graph G. An example of a graph and its distance spectrum are given in Figure 1. From matrix theory (see *e.g.* [42, Theorem 0.2 and 0.3]) and since $\mathcal{D}$ is an irreducible, non–negative, real and symmetric matrix, ∂_1 is a simple eigenvalue and satisfies $\partial_1 \geq |\partial_i|$, for $i = 2, 3, \ldots, n$, and there exists a positive eigenvector corresponding to ∂_1. The largest eigenvalue ∂_1 is called the *distance spectral radius* or *distance index*. The index of $\mathcal{D}$ is the most studied among the distance eigenvalues.

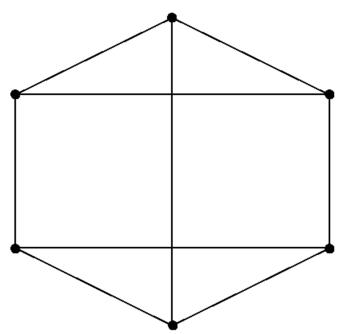

Figure 1: A graph with a distance spectrum $\{7, 0, 0, -2, -2, -3\}$.

The *Wiener index* $W(G)$ of a graph is the sum of the distances between all unordered pairs of vertices of G, in other words $W(G)$ is half the sum of all the entries of the distance matrix of G, *i.e.*,

$$W(G) = \sum_{1 \leq i < j \leq n} \mathcal{D}_{i,j}.$$

The *transmission* $Tr(v)$ of a vertex v in G is the sum of the distances from v to all other vertices in G, *i.e.*,

$$Tr(v) = \sum_{u \in V} d(u, v).$$

Note that the transmission of a vertex is the sum of the entries of $\mathcal{D}$ in the column (row) corresponding to v. For short, we write Tr_i for $Tr(v_i)$, when the vertices are labeled. We say that G is a k–transmission regular graph if $Tr(v) = k$ for every $v \in V$. Note that there exist graphs which are transmission regular but not (degree) regular. Indeed, the graph on 9 vertices illustrated in Figure 2 is 14–transmission regular but not degree regular. For more examples of transmission regular but not degree regular graphs see [5, 7].

The remainder of the present paper is organized as follows. In the next section, we give an overview of the first papers devoted to the distance spectra of graphs. These papers deal mainly with the distance characteristic polynomials and their coefficients, and the problem of characterizing the graphs whose distance spectra contain exactly one positive eigenvalue. Section 3 is devoted to the results related to the entries of the Perron vector. In Section 4, we report on the distance spectra of some particular classes of graphs; the distance

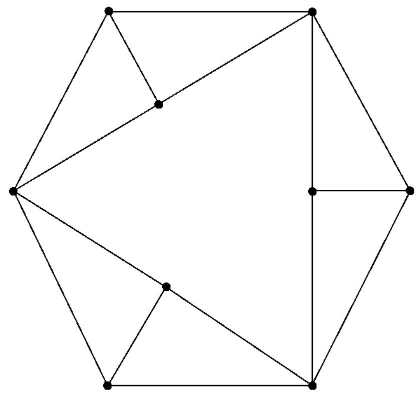

Figure 2: The smallest transmission regular but not degree regular graph.

characteristic polynomial of a graph obtained by means of operations involving two graphs or more; the behavior of some distance eigenvalues, especially the distance spectral radius, when some transformations are done on the graph. Section 5 is devoted to results involving the distance spectral radius, such as lower and upper bounds over the class of graphs with given order n. Results related to the distance spectral spread are presented in Section 6. The papers dealing with the distance energy (the sum of the absolute values of the distance eigenvalues) are overviewed in Section 8.

2 The distance matrix and its characteristic polynomial

Among the first results related to the distance matrix figures the remarkable theorem proved by Graham and Pollack [64] that gives a formula for the determinant of the distance matrix of a tree depending only on the order n.

Theorem 2.1 ([64]) *If T is a tree on $n \geq 2$ vertices with distance matrix $\mathcal{D}$, then*

$$Det(\mathcal{D}) = (-1)^{n-1}(n-1)2^{n-2}.$$

The generalization of the above theorem for general graphs is that the determinant of the distance matrix depends only on the *blocks* of the graph. This generalization was first conjectured by Hosoya, Murakami and Gotoh [74] and then proved by Graham, Hoffman and Hosoya [61]. Before the statement of the result recall the following definitions. A graph that has no cut vertices is called a *block*. A *block of a graph* is a subgraph that is a block and maximal with respect to this property. Every graph is the union of its blocks. For a square matrix M, denote by $cof(M)$ the sum of its cofactors.

Theorem 2.2 ([61]) *If G is a (strongly connected directed) graph with blocks $G_1, G_2, \ldots G_k$, then*

$$cof(\mathcal{D}(G)) = \prod_{i=1}^{k} cof(\mathcal{D}(G_i)) \quad \text{ and } \quad det(\mathcal{D}(G)) = \sum_{i=1}^{k} det(\mathcal{D}(G_i)) \prod_{i=1, j\neq i}^{k} cof(\mathcal{D}(G_j)).$$

The *inertia* of a square matrix M with real eigenvalues is the triplet $(n_+(M), n_0(M), n_-(M))$, where $n_+(M)$ and $n_-(M)$ denote the number of positive and negative eigenvalues of M, respectively, and $n_0(M)$ is the (algebraic) multiplicity of 0 as an eigenvalue of M.

An immediate consequence of Theorem 2.1 is that the inertia of the distance matrix is the same for all trees on $n \geq 2$ vertices.

Corollary 2.3 ([64]) *If T is a tree on $n \geq 2$ vertices with distance matrix $\mathcal{D}$, then the inertia of $\mathcal{D}$ is* $(1, 0, n-1)$.

The above corollary is related to and stated in the context of the addressing problem in communication systems.

Consider the characteristic polynomial of $\mathcal{D}$ of a tree T on n vertices,

$$P_{\mathcal{D}(T)}(t) = \sum_{k=0}^{n} a_k t^k.$$

The determinant of $\mathcal{D}$ is given by the distance characteristic polynomial at 0, *i.e.*, $Det(\mathcal{D}) = (-1)^n P_{\mathcal{D}}(0) = (-1)^n a_0$. Considering this point of view, Theorem 2.1 gives the value of a coefficient of the distance characteristic polynomial. Thus, the study of the coefficients of $P_{\mathcal{D}}$ is a natural extension of the work done in [64]. Edelberg, Garey and Graham [55], and Graham and Lovász [62] were the first authors to do such extensions. Edelberg, Garey and Graham [55] computed some coefficients and determined the sign of each coefficient. In order to state the next results, we recall the following notations. The unique tree on 5 vertices with a diameter $D = 3$ is denote by Y. For a given tree T and a subtree H, $N_H(T)$ denotes the number of subtrees of G isomorphic to H. As usual, $sgn(t)$ denotes the sign of a real number t.

Theorem 2.4 ([55]) *For any tree on n vertices, we have*

$$\begin{aligned}
&sgn(a_k) = (-1)^{n-1}, \text{ for } 0 \le k \le n-2,\\
&a_{n-1} = 0,\\
&a_n = (-1)^n,\\
&a_{n-2} = (-1)^{n-1}\sum_{i<j} d_{ij}^2,\\
&a_{n-3} = (-1)^{n-1}\sum_{i<j<k} d_{ij}d_{jk}d_{ki},\\
&a_k \equiv 0 (mod\ 2^{n-k-2}) \qquad \text{for } 0 \le k \le n-2\\
&a_0 = (-1)^{n-1}2^{n-2}N_{S_2}(T),\\
&a_1 = (-1)^{n-1}2^{n-3}\left(2nN_{S_2}(T) - 2N_{S_3}(T) - 4\right),\\
&a_2 = (-1)^{n-1}2^{n-4}\left(2(n^2-n-4)N_{S_2}(T) - (5n-7)N_{S_3}(T) + 6N_{S_4}(T) - 2N_{P_3}(T)\right),\\
&a_3 = (-1)^{n-1}2^{n-5}\Big[\frac{4}{3}(n^2-4)(n-3)N_{S_2}(T) - 2(3n^2-11n+9)N_{S_3}(T) + 2(7n-22)N_{S_4}(T)\\
&\qquad -4(n-3)N_{P_3}(T) - 2N_{P_4}(T) - 24N_{S_5}(T) + 4N_Y(T) + 2(N_{S_3}(T))^2\Big].
\end{aligned}$$

Note that the results in the above theorem, except $sgn(a_k)$ and a_3, have been found independently by Hosoya, Murakami and Gotoh [74].

In [62], Graham and Lovász showed, in a generalization of the above theorem, that the coefficients of the distance characteristic polynomial of a tree T depend only on the number of occurrences of subforests of T.

Theorem 2.5 ([62]) *Let T be a tree on $n \ge 2$ vertices. The coefficients of the distance characteristic polynomial of T can be written in the form*

$$a_k = (-1)^{n-1}2^{n-k-2}\sum_F A_F^{(k)} N_F(T),$$

where F ranges over all subforests of T with $k-1$, k or $k+1$ edges and no isolated vertices, and $A_F^{(k)}$ is an integer depending only on k and F.

Explicit formulas for the integers $A_F^{(k)}$ are given in [62]. They turn out to depend only on the number of occurrences of various paths in the connected components of F.

The above theorem was generalized to the case of weighted trees by Collins in [38].

In [62], Graham and Lovász conjectured that the sequence of the distance characteristic polynomial is unimodal with the maximum value occurring for $k = \lfloor n/2 \rfloor$. Collins [37] confirmed the conjecture for the star S_n and showed that, in the case of a path P_n, the sequence is unimodal with a maximum value at $\left(1 - 1/\sqrt{5}\right) n$. Thus, Collins [37] reformulated the conjecture as follows.

Conjecture 2.6 ([37]) *The coefficients of the distance characteristic polynomial of any tree T with n vertices are unimodal with peak between $n/2$ and $\left(1 - 1/\sqrt{5}\right) n$.*

No more results are known about that conjecture.

The problem of finding the coefficients of the characteristic polynomial of the distance matrix was also studied by Mihalić et al. [101] in the context of the use of the distance matrix in Chemistry. Computer programs for calculating the distance characteristic polynomials of graphs were developed by Balasubramanian [10, 11].

The first application of the distance eigenvalues was expressed in terms of the number of positive and negative eigenvalues $n_+(G)$ and $n_-(G)$, respectively, of a graph $G = (V, E)$. Suppose one wishes to label each vertex v of G with an N-tuple $A(v) = (a_1, a_2, \ldots, a_N)$, where $a_i \in \{0, 1, *\}$, so that

$$d(A(v), A(v')) = d_G(v, v') \qquad \text{for all } v, v' \in V,$$

and where $d_G(v, v')$ denotes the distance between v and v' in G, and $d(A(v), A(v')) = |\{i : \{a_i, a_{i'}\} = \{0, 1\}\}|$ (also called Hamming distance). Such a labeling exists for any simple connected graph, provided N is large enough. The problem is to determine the smallest $N = N(G)$ satisfying that property. The following result is proved in [64].

Theorem 2.7 ([64]) *For any graph G, we have*

$$N(G) \geq \max\{n_+(G), n_-(G)\}.$$

Graham and Lovász [62] proved that it is possible to compute the inverse of the distance matrix of a tree in terms of the degrees and the entries of the adjacency matrix.

Theorem 2.8 ([62]) *If T is a tree on $n \geq 2$ vertices with distance matrix $\mathcal{D} = (d_{ij})$, then the inverse matrix of $\mathcal{D}$, $\mathcal{D}^{-1} = \left(d_{ij}^{(-1)}\right)$ is given by*

$$d_{ij}^{(-1)} = \frac{(2 - d_i)(2 - d_j)}{2(n-1)} + \begin{cases} -\frac{d_i}{2} & \text{if } i = j \\ \frac{a_{ij}}{2} & \text{if } i \neq j, \end{cases}$$

where d_i denotes the degree of the vertex v_i and $A = (a_{ij})$ is the adjacency matrix of T.

Theorem 2.1 and Theorem 2.8 were generalized to the case of trees with attached graphs (trees with graphs defined on its partitions) by Bapat [15], and to the case of weighted trees by Collins [38], and Bapat, Kirkland and Neumann [16]. Since the formulae in [15] are the same as in [62, 64], we only recall the results related to weighted trees.

Theorem 2.9 ([16, 38]) *Let T be a weighted tree on n vertices with edge weights $\alpha_1, \alpha_2, \ldots, \alpha_{n-1}$ and let $\mathcal{D}$ be the corresponding distance matrix. Let L denote the Laplacian matrix for the weighting of T that arises by replacing each edge weight by its reciprocal. For each $i = 1, \ldots, n$, let d_i be the degree of the vertex i, let $\delta_i = 2 - d_i$, and set $\delta = [\delta_1, \ldots, \delta_n]^T$. Then*

$$\mathcal{D}^{-1} = -\frac{1}{2} L + \frac{1}{2\sum_{i=1}^{n-1} \alpha_i} \delta\delta^T. \tag{1}$$

Observe that using the notation defined in Theorem 2.9, the inverse defined in Theorem 2.8 can be written as

$$\mathcal{D}^{-1} = -\frac{1}{2} L + \frac{1}{2(n-1)} \delta\delta^T,$$

and then the generalization becomes clear. Note also that Theorem 2.9 is formulated in [38] using a notation similar to that of Theorem 2.8.

The second generalization concerns the determinant of the distance matrix, however instead of calculating it in a straightforward way, the authors of [16] first proved more general results and then deduced the determinant. These are the results and then the determinant as a corollary.

Theorem 2.10 ([16]) *Let G be a t–transmission regular and weighted graph on n vertices with distance matrix $\mathcal{D}$. Form G^* from G by adding weighted branches to G on a total of p new vertices, with positive weights $\alpha_1, \ldots, \alpha_p$ on the new edges. Let $\mathcal{D}^*$ be the distance matrix for G^*. Then for each $x \in IR$,*

$$det(\mathcal{D}^* + xJ) = (-2)^p det(\mathcal{D}) \left(\prod_{i=1}^{p} \alpha_i\right) \left(1 + \frac{nx}{t} + \frac{n}{2t}\sum_{i=1}^{p} \alpha_i\right).$$

Further, $n_0(\mathcal{D}) = n_0(\mathcal{D}^*)$ and if, in addition, $\mathcal{D}$ is non–singular, then $n_+(\mathcal{D}) = n_+(\mathcal{D}^*)$.

Theorem 2.11 ([16]) *Let T be a weighted tree on $n \geq 2$ vertices with edge weights α_i, for $i = 1, \ldots, n-1$. Let $\mathcal{D}$ be the distance matrix of T. Then for any real number x,*

$$det(\mathcal{D} + xJ) = (-1)^{n-1} 2^{n-2} \left(\prod_{i=1}^{p} \alpha_i\right) \left(2x + \sum_{i=1}^{p} \alpha_i\right).$$

Further, the inertia of $\mathcal{D}$ is $(n_+(\mathcal{D}), n_0(\mathcal{D}), n_-(\mathcal{D})) = (1, 0, n-1)$.

The result about the inertia of $\mathcal{D}$ in the above theorem was also given in [14]. The next result was first proved in [14, 38] and then obtained in [16] as a corollary from the above theorem.

Corollary 2.12 ([14, 16, 38]) *Let T be a weighted tree on n vertices with edge weights α_i, for $i = 1, \ldots, n-1$. Let $\mathcal{D}$ be the distance matrix of T. Then*

$$det(\mathcal{D}) = (-1)^{n-1} 2^{n-2} \left(\prod_{i=1}^{n-1} \alpha_i\right) \left(\sum_{i=1}^{n-1} \alpha_i\right).$$

Bapat, Kirkland and Neumann [16] extended their results about the distance matrix of a tree to that of a *unicyclic* graph, *i.e.*, a connected graph containing exactly one cycle. The first result they proved is a formula for the inverse of the distance matrix of an odd cycle.

Theorem 2.13 ([16]) *Let $\mathcal{D}$ be the distance matrix for the cycle on $2k+1$ vertices. Then*

$$\mathcal{D}^{-1} = -2I - C^k - C^{k+1} + \frac{2k+1}{k(k+1)} J$$

where C is the cyclic permutation matrix of order $2k+1$ having $C_{i,i+1} = 1$ for $i = 1, \ldots, 2k+1$, taking indices modulo $2k+1$.

An immediate corollary of the above theorem is the following result about the spectrum of an odd cycle.

Corollary 2.14 ([16]) *The distance matrix for a cycle on $2k+1$ vertices has exactly one positive eigenvalue.*

They [16] also calculated the determinant, as well as the inertia, of the distance matrix of a unicyclic graph with an odd cycle.

Theorem 2.15 ([16]) *Let G be a unicyclic graph on $2k+1+p$ vertices and cycle length $2k+1$. Let $\mathcal{D}$ be the distance matrix of G. Then*

$$det(\mathcal{D}) = (-2)^p \left(k(k+1) + \frac{(2k+1)p}{2}\right),$$

while the inertia of $\mathcal{D}$ is given by $(n_+(\mathcal{D}), n_0(\mathcal{D}), n_-(\mathcal{D})) = (1, 0, 2k+p)$.

The inertia of a unicyclic graph with an even cycle is as follows.

Theorem 2.16 ([16]) *Let G be a unicyclic graph on $2k+p$ vertices with an even cycle of length $2k$. Let $\mathcal{D}$ be the distance matrix of G. Then the inertia of $\mathcal{D}$ is $(n_+(\mathcal{D}), n_0(\mathcal{D}), n_-(\mathcal{D})) = (1, k-1, k+p)$.*

Note that to prove the above theorem, Bapat, Kirkland and Neumann [16] used the following lemma.

Lemma 2.17 ([16]) *Let G_0 be a graph with distance matrix $\mathcal{D}_0$ and suppose that for all $x > 0$, $\mathcal{D}_0 + xJ$ has a single positive eigenvalue (namely the Perron value). Form G_p from G_0 by adding unweighted branches at various vertices of G_0, on a total of p new vertices. If $\mathcal{D}$ is the corresponding distance matrix, then $\mathcal{D}_p + xJ$ has just one positive eigenvalue for any $x > 0$.*

Corollary 2.3 stated that trees have exactly one positive distance eigenvalue. This fact motivated the search and study of graph families having one positive distance eigenvalue. Ramane et al. [112] stated sufficient conditions on a graph such that its *line graph* $L(G)$ has exactly one positive distance eigenvalue. First, recall the following definition. Let G be a graph. The *line graph* $L(G)$ of G is the graph whose vertices correspond to the edges of G with two vertices of $L(G)$ being adjacent if and only if the corresponding edges in G have a vertex in common. For instances, the line graph of a cycle on n vertices is a cycle on n vertices, *i.e.*, $L(C_n) \cong C_n$; the line graph of a path on n vertices is a path on $n-1$ vertices, *i.e.*, $L(P_n) \cong P_{n-1}$; and the line graph of a star on n vertices is the clique on $n-1$ vertices, *i.e.*, $L(S_n) \cong K_{n-1}$.

Theorem 2.18 ([112]) *If G is a k–regular graph on n vertices with diameter $D \leq 2$ such that none of the graphs F_1, F_2 and F_3 (Figure 3) is an induced subgraph of G, then $L(G)$ has exactly one positive distance eigenvalue $\partial_1(L(G)) = k(n-2)$.*

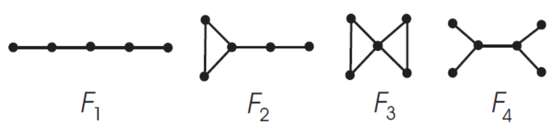

Figure 3: Some forbidden graphs.

The next corollary follows from and generalizes, in some way, the above theorem.

Corollary 2.19 ([112]) *Let G be a k–regular graph on n vertices with diameter $D \leq 2$ and let none of the four graphs of Figure 3 be an induced subgraph of G. Let n_p and k_p be the order and degree, respectively, of the p–th iterated line graph $L^p(G)$ of G, $p \geq 1$. Then $L^p(G)$ has exactly one positive distance eigenvalue*

$$\partial_1(L^p(G)) = n_{p-1}k_{p-1} - 2k_{p-1} = 2n_p - k_p - 2 = 2n\prod_{i=1}^{p-1}(2^{i-1}k - 2^i + 1) - (2^p k - 2^{p+1} + 4)$$

Let $G = (V, E)$ be a graph. Let i, j, k be non–negative integers. $G = (V, E)$ is called *distance–regular* if for any choice of $u, v \in V$ with $d(u, v) = k$, the number of vertices $w \in V$ such that $d(u, w) = i$ and $d(v, w) = j$ is independent of the choice of u and v. All the cubic (3–degree regular) distance–regular graphs on at most 10 vertices are illustrated in Figure 4. For more details about distance–regular graphs see the book [25].

All the distance–regular graphs that have exactly one distance positive eigenvalue are characterized by Koolen and Shpectorov [90]. We first define the graphs and then state the result. The *cocktail party graph* CP_k on $2k$ vertices, also called the *hyperoctahedral graph* [17], is the graph obtained from the complete graph K_{2k} by the deletion of k disjoint edges, *i.e.*, the complement of the graph consisting of k disjoint edges. See Figure 7 for an illustration of the cocktail party graph CP_3. The *Gosset graph* (see *e.g.* [25]) has as vertices all the vectors of length 8, either consisting of two 1's and six 0's, or consisting of six $\frac{1}{2}$ and two $-\frac{1}{2}$; e.g. $(1, 1, 0, 0, 0, 0, 0, 0)$, $(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ are vertices of the Gosset graph. Two vertices are adjacent if and only if their inner product is exactly 1 (so the first and the second, as well as the second and the third vector of the above three are adjacent). See Figure 5 for a projection of the Gosset

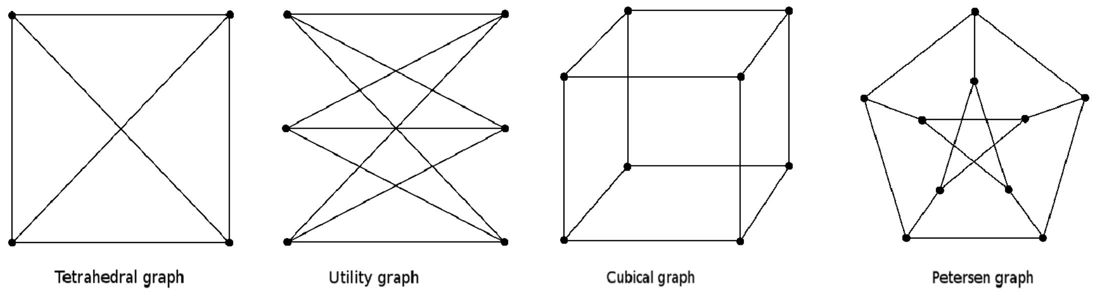

Figure 4: All the cubic distance–regular graphs on at most 10 vertices.

graph on a plane. The *Schläfli graph* (see *e.g.* [25]) is the subgraph of the Gosset graph consisting of the $(0,1)$–vectors with one 1 at the last two places and the $(\frac{1}{2},-\frac{1}{2})$–vectors with minus signs at the first six places only. The Schläfli graph is illustrated in Figure 6. Let Q_k be the k–cube and let $V_1 \cup V_2$ be its bipartition as a bipartite graph. Then the *halved cube* Q'_k ([25]) is the graph with $V(Q'_k) = V_1$, where u is adjacent to v in Q'_k if and only if $d_{Q_k}(u,v) = 2$. Clearly, Q'_k has 2^{k-1} vertices and is $(k(k-1)/2)$–regular. Note that Q'_3 is isomorphic to K_4 and that Q'_4 is isomorphic to the cocktail party graph on 8 vertices. The *Johnson graph* $J(n,k)$ is defined on the set of vertices composed of the k–element subsets of an n–element set, and where two vertices are adjacent if and only they share $k-1$ elements. For instances, $J(n,1)$ is the complete graph K_n, $J(4,2)$ is the tripartite graph $K_{2,2,2}$; and $J(5,2)$ is the complement graph of the Petersen graph or equivalently the line graph of K_5. A k–regular graph G on n vertices is said *strongly regular* if there exist two integers p and q such that any two adjacent vertices in G have p common neighbors and any non adjacent vertices have q common neighbors. In this case n, k, p and q are the called the parameters of G, and then we speak about an (n,k,p,q)–strongly regular graph. There are exactly four $(28,12,6,4)$–strongly regular graphs, one of which is the line graph of the complete graph K_8 and the three others are known as *Chang graphs*. The Chang graphs are implemented in *Mathematica* as "GraphData[{"Chang" , n}]" for $n = 1,2,3$.

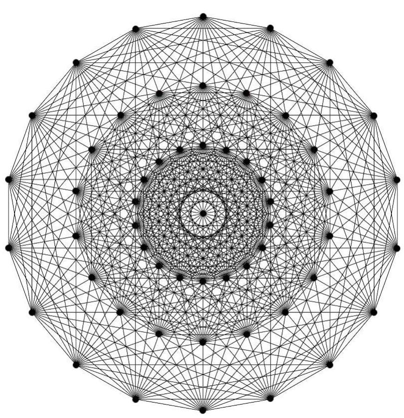

Figure 5: A projection of the Gosset graph. Note that two vertices coincide in the center of this graph. Edges also coincide with this projection.

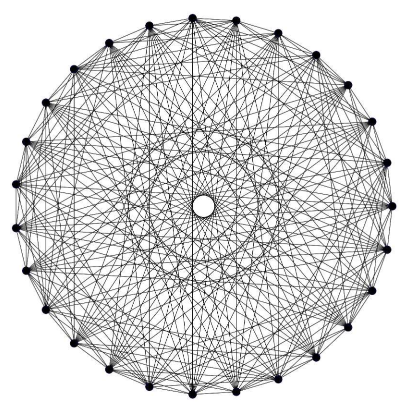

Figure 6: The Schläfli graph.

The *Cartesian product* $G_1 \square G_2$ of two graphs G_1 and G_2 is the graph whose vertex set is the (set) Cartesian product $V(G_1) \times V(G_2)$, and in which two vertices (u,u') and (v,v') are adjacent if and only if either $u = v$ and u' is adjacent with v' in G_2, or $u' = v'$ and u is adjacent with v in G_1.

The *Hamming graph* $H(D,p)$, $D \geq 2$ and $p \geq 2$, of diameter D and characteristic p is the graph whose vertex set consists of all D-tuples of elements taken from a p–element set, in which two vertices are adjacent if and only if they differ in exactly one coordinate. $H(D,p)$ can also be defined as the Cartesian product of the

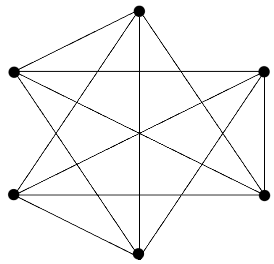

Figure 7: The cocktail party graph CP_3.

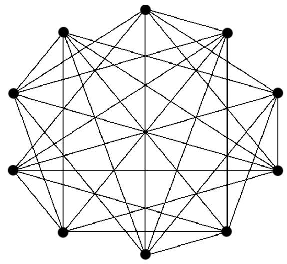

Figure 8: The Johnson graph $J(5, 2)$.

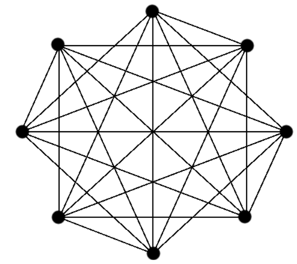

Figure 9: The halved cube Q'_8.

complete graph K_p by itself D times, *i.e.*,

$$H(D,p) = \underbrace{K_p \square K_p \square \cdots \square K_p}_{D \text{ times}}.$$

The *Shrikhande graph* is the graph whose vertex set is $\{0,1,2,3\} \times \{0,1,2,3\}$ and in which two vertices (a,b) and (c,d) are adjacent if and only if $(a,b) - (c,d) \in \{\pm(0,1), \pm(1,0), \pm(1,1)\}$. A *Doob graph* $D(m,n)$ is the Cartesian product of m copies of the Shrikhande graph and the Hamming graph $H(n,4)$.

A *double odd graph* DO_k is a graph whose vertices are k–element or $(k+1)$–element subsets of a $(2k+1)$–element set, where two vertices u and v are adjacent if and only if $u \subset v$ or $v \subset u$, as subsets.

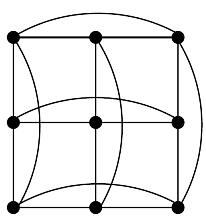

Figure 10: The Hamming graph $H(2, 3)$.

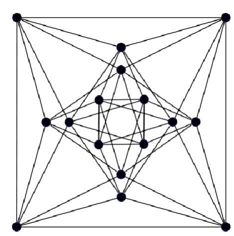

Figure 11: The Shrikhande graph.

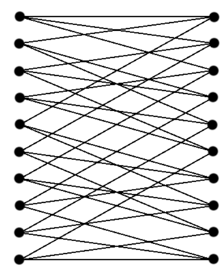

Figure 12: The double odd graph DO_2.

Theorem 2.20 ([90]) *Let G be a distance–regular graph. The distance matrix of G has exactly one positive eigenvalue if and only if G is one of the following graphs: a cocktail party graph; the Gosset graph; the Schläfli graph; a halved cube; a Johnson graph; one of the three Chang graphs; a Hamming graph; a Doob graph; the icosahedron (see Figure 13); a polygon (cycle); a double odd graph; the Petersen graph (see Figure 4); the dodecahedron (see Figure 14).*

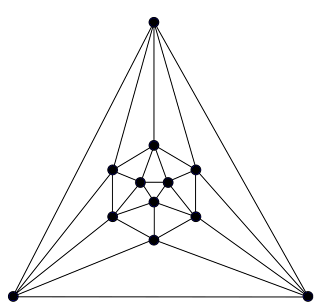

Figure 13: The icosahedron.

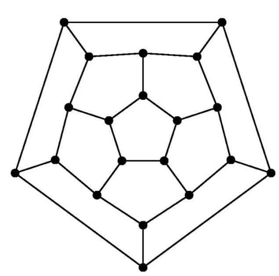

Figure 14: The dodecahedron.

In [100], Merris studied the distance spectrum of a tree with a given number of vertices. In order to estimate the distance eigenvalues of a tree on n vertices and $m = n-1$ edges, he associated the matrix $K = K(T) = Q^TQ = 2I_m + A(T^*)$ to the tree T, where Q is the incidence matrix of T (arbitrarily oriented), I_m is the unit $m \times m$–matrix, and $A(T^*)$ denotes the adjacency matrix of the line graph T^* of T. Note the similarity between the matrix K and the Laplacian of T defined by $L(T) = QQ^T = Diag(T) - A(T)$. The main result proved in [100] is the following:

Theorem 2.21 ([100]) *Let T be a tree. Then the eigenvalues of $-2K^{-1}$ interlace the distance eigenvalues of T.*

To prove the above theorem, the following lemma was used.

Lemma 2.22 ([100]) *If T is a tree on n vertices and $m = n-1$ edges, then $Q^T\mathcal{D}Q = -2I_m$, where $\mathcal{D}$ denotes the distance matrix of T.*

A *pendent vertex* (also written *pendant vertex*) of T is a vertex of degree 1. A *pendent neighbor* is a vertex adjacent to a pendent vertex. Suppose T has n_1 pendent vertices and n_1' pendent neighbors. A series of corollaries for Theorem 2.21 were proved and they are gathered below.

Corollary 2.23 ([100]) *Let T be a tree with n_1 pendent vertices and n_1' pendent neighbors.*

- *Let ∂ be a distance eigenvalue of T of multiplicity k. Then $k \leq n_1$.*
- *Among the distance eigenvalues of T, $\partial = -2$ occurs with multiplicity at least $n_1 - n_1' - 1$.*
- *If D denotes the diameter of T, then*

$$
\begin{array}{ll}
(i) & \partial_n \leq \dfrac{-1}{1-\cos\left(\frac{\pi}{D+1}\right)};\\
(ii) & \partial_{\lfloor \frac{D}{2} \rfloor} > -1;\\
(iii) & \partial_{n_1'} > -1 \qquad \textit{(provided } n > 2n_1'\textit{);}\\
(iv) & \partial_{n-n_1'+2} < -2;\\
(v) & \partial_{n_1+2} \geq -2;\\
(vi) & \partial_{n-n_1+2} \leq -2.
\end{array}
$$

The second point of the above corollary was improved by Collins [36].

Theorem 2.24 ([36]) *Let T be a tree with n_1 pendent vertices and n_1' pendent neighbors. Then, among the distance eigenvalues of T, $\partial = -2$ occurs with multiplicity at least $n_1 - n_1'$.*

In some cases, it is possible to deduce some graph eigenvalues from the graph structure. It is the case for the distance matrix whenever the graph contains two vertices sharing the same neighborhood, as proved in the next theorem.

Theorem 2.25 ([91]) *If there are two vertices with the same neighborhood in a graph G, then one root of the distance polynomial is either -1 (if the two vertices are adjacent) or -2 (if the two vertices are not adjacent).*

The results gathered in the next theorem and dealing with the characteristic polynomial of the distance matrix of a graph, were proved by McKay in [99]. First, recall that the *cone* $\hat{G}$ of a graph G is the graph obtained from G by adding a new vertex joined to each vertex of G.

Theorem 2.26 ([99]) *Let G be a graph on n vertices.*

- *If G is a tree, then*

$$P_{\mathcal{D}}(x) = -\frac{x^n}{4} \cdot \left[P_{L^*}\left(\frac{2}{x}\right) + \left(n - 1 - \frac{2}{x}\right) \cdot P_{-L}\left(\frac{2}{x}\right) \right],$$

where L is the Laplacian matrix of G and L^* is the symmetric $(n+1) \times (n+1)$–matrix obtained from L by adding, as the first row and first column, the $(n+1)$–vector q with $q_1 = 0$ and $q_{i+1} = 2 - d_i$ for $i = 1, \ldots, n$.

- *If $\overline{G}$ has diameter 2, then*

$$P_{\mathcal{D}(\overline{G})}(x) = P_{\hat{A}}(x+1) - xP_A(x+1),$$

where $\hat{A}$ denotes the adjacency matrix of the cone graph of G.

In the same paper, McKay [99] studied the problem of finding cospectral but non–isomorphic graphs. He constructed an infinite family of pairs of cospectral but non–isomorphic trees. A pair of these trees is given in Figure 15. First, we recall the definition of an operation on two trees. Let S and T be two rooted trees on $m_1 + 1$ and $m_2 + 1$ vertices respectively. The *coalescence* $S \bullet T$ of S and T is the $(m_1 + m_2 + 1)$–vertex tree formed by identifying the roots of S and T. The rooted trees S and T are called *limbs* of $S \bullet T$.

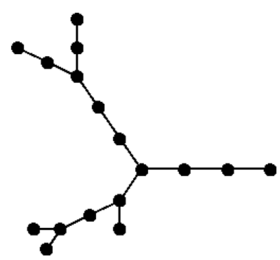

Figure 15: The smallest two cospectral non–isomorphic trees (on 17 vertices).

Theorem 2.27 ([99]) *Let $S_i = S \bullet T_i$ for $i = 1, 2$, where S is any rooted tree on at least two vertices and T_1 and T_2 are the trees of Figure 16 rooted at the white vertices. Then, S_1 and S_2 are not isomorphic and*

$$P_{\mathcal{D}(S_1)}(x) = P_{\mathcal{D}(S_2)}(x) \qquad \text{and} \qquad P_{\mathcal{D}(\overline{S}_1)}(x) = P_{\mathcal{D}(\overline{S}_2)}(x).$$

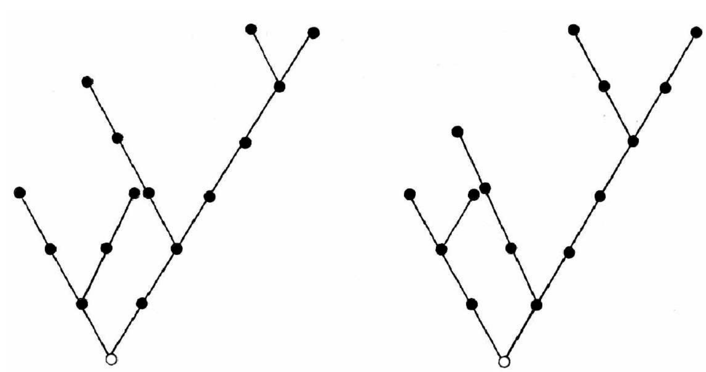

Figure 16: The trees T_1 and T_2 of Theorem 2.27.

McKay [99] also studied the proportion of trees on n vertices that can be characterized by their characteristic polynomial.

Theorem 2.28 ([99]) *Let $p(n)$ be the proportion of the trees on n vertices which are characterized (amongst trees) by the characteristic polynomial of their distance matrix or that of their complements. Then $p(n) \to 0$ as $n \to \infty$.*

Despite the fact proved in the above theorem, it seems that the distance spectral radius determines the spectrum of a tree. Stevanović and Indulal [132] experimentally confirmed it for all trees on at most 22 vertices, and for all chemical trees (trees with maximum degree at most 4) on at most 24 vertices. Then they suggested the following conjecture.

Conjecture 2.29 ([132]) *There exist no two distance non–cospectral trees T_1 and T_2 with $\partial_1(T_1) = \partial_1(T2)$.*

3 The Perron vector of the distance matrix

In this section, we give a survey of the results related to (the entries of) the Perron vector of the distance matrix. By the Perron–Frobenius theorem, the distance spectral radius ∂_1 has a unique unit positive eigenvector x, called the *Perron vector* or *principal eigenvector* (sometimes it is not required to be a unit vector, in which case, it is not unique).

Let $G = (V, E)$ be a graph containing a bridge (an edge whose removal disconnects the graph) $e = uv$. Let $V_u = \{w \in V : d(u, w) < d(v, w)\}$ and $V_v = \{w \in V : d(v, w) < d(u, w)\}$. In fact V_u and V_v define a partition of V and are the vertex sets of the connected components of $G - e$ containing u and v respectively. The first result in this section provides a relationship between the sum of the Perron vector entries over V_u and the sum of those over V_v.

Theorem 3.1 ([130, 131]) *Let G be a graph containing a bridge $e = uv$. Let x be the distance principal eigenvector of G. Assume that the entries of x are indexed by the vertices of G. Then*

$$\partial_1 \cdot (x_u - x_v) = \sum_{w \in V_v} x_w - \sum_{w \in V_u} x_w = \sum_{w \in V} x_w - 2 \sum_{w \in V_u} x_w.$$

The next result is about the Perron vector entries corresponding to three vertices forming two consecutive edges one of which is a bridge.

Theorem 3.2 ([116]) *Let v_{i-1}, v_i and v_{i+1} be vertices in a graph G such that $v_{i-1}v_i, v_iv_{i+1} \in E(G)$, and let x be the Perron vector of G. If $x_{i-1} < x_i$ and one of the edges $v_{i-1}v_i$ and v_iv_{i+1} is a bridge, then $x_i < x_{i+1}$.*

The proof of the above theorem led to the next result.

Corollary 3.3 ([116]) *If v_{i-1} is a pendant vertex attached to a vertex v_i, then $x_{i-1} > x_i$.*

For the particular case of a tree, and since any of its edges is a bridge, Theorem 3.2 is stated as follows.

Theorem 3.4 ([116]) *Let T be a tree on $n \geq 3$ vertices with a Perron vector x. If $x_{i-1} < x_i$, then the entries of x along any path of the form $v_{i-1}v_i \cdots$ form an increasing sequence of positive numbers.*

As a corollary of the above theorem, Ruzieh and Powers [116] stated

Corollary 3.5 ([116])

- *For a tree, the minimum value among the Perron vector entries occurs at an interior vertex. Moreover, this minimum may occur at two vertices at most, in which case they are adjacent.*
- *For a tree, the maximum value among the Perron vector entries occurs at a pendant vertex and may occur at several vertices.*

Let G be a graph and v a vertex in G. For $k \geq 1$, denote by $G(v, k)$ the graph obtained from $G \cup P_k$ by adding an edge between v and an endpoint of P_k. For such a graph, we have the following result.

Theorem 3.6 ([131]) *Let x be the Perron vector of $G(v, k)$, $k \geq 1$, and ∂_1 the distance spectral radius of $G(v, k)$. Denote by x_0 the component of x at v and $x_1, x_2, \ldots, x_k$ the components of x along P_k starting from the endpoint adjacent to v. Then, there exist constants a and b depending on ∂_1, x_0, k and the sum of the entries of x such that*

$$x_i = at^i + bs^i, \qquad \text{for} \quad 0 \leq i \leq k,$$

where

$$t = 1 + \frac{1}{\partial_1} - \frac{\sqrt{2\partial_1 + 1}}{\partial_1} \qquad \text{and} \qquad s = 1 + \frac{1}{\partial_1} + \frac{\sqrt{2\partial_1 + 1}}{\partial_1}.$$

The next two theorems are stated for the entries of the Perron vector of the distance matrix of a graph that contains (at least) two pending paths.

Consider the graph $G(v,k,l)$ obtained from a graph G on at least two vertices and two paths P_k and P_l by joining one endpoint of each path to a fixed vertex v from G (see Figure 17), where k and l are two integers.

Theorem 3.7 ([131]) *Let x be the Perron vector of $G(v,k,l)$, $k,l \geq 1$ and ∂_1 the distance spectral radius of $G(v,k,l)$. Denote by x_0 the component of x at v, $x_1, x_2, \ldots, x_k$ the components of x along P_k starting from the endpoint adjacent to v, and $y_1, y_2, \ldots, y_l$ the components of x along P_l starting from the endpoint adjacent to v (see Figure 17). If $k \geq l$, then*

$$\sum_{i=1}^{k} x_i \geq \sum_{i=1}^{l} y_i.$$

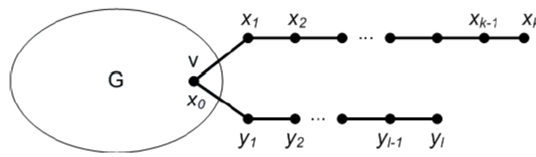

Figure 17: The graph of Theorem 3.7.

Zhang and Godsil [149] proved that the above result remains true if the vertex v is replaced by an edge in which each end vertex is an endpoint of one of the attached paths (see Figure 18).

Theorem 3.8 ([149]) *Let v_k and v_l be two adjacent vertices of a graph G. Let P_k and P_l be two paths attached to G at v_k and v_l, respectively. If $k > l$, then*

$$\sum_{i \in V(P_k)} x_i > \sum_{i \in V(P_l)} x_i.$$

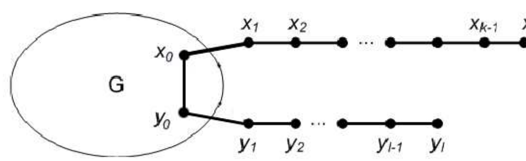

Figure 18: The graph of Theorem 3.8.

The above theorems are stated for graphs with attached paths. If instead of two attached paths we have two sets of pendent vertices to the endpoints of a path, then the components of the Perron vector are also comparable. The related result was proved by Yu, Jia, Zhang and Shu [143].

Theorem 3.9 ([143]) *Let G be the graph obtained by attaching pendent vertices v_{n-r+1}, v_{n-r+2}, $\ldots$, v_{n-r+s} to the vertex v_1 of a path $P = v_1 v_2 \cdots v_{n-r}$ and attaching pendent vertices $v_{n-r+s+1}$, $v_{n-r+s+2}$, $\ldots$, v_n to the vertex v_{n-r}. Let $X = (x_1, x_2, \ldots, x_n)^T$ be the Perron eigenvector corresponding to $\partial_1(G)$, in which x_i corresponds to v_i. Let*

$$S_1 = \sum_{i=n-r+1}^{n-r+s} x_i \qquad \textit{and} \qquad S_2 = \sum_{i=n-r+s+1}^{n} x_i.$$

If $s \geq p$, then $S_1 \geq S_2$, but $x_{n-r+1} \leq x_{n-r+s+1}$. In particular, $x_{n-r+1} > x_{n-r+s+1}$ if $s > p$.

In a graph G, if the neighborhood of a vertex contains the neighborhood of another vertex, then the entries of the Perron vector of $\mathcal{D}(G)$ corresponding to the two vertices are comparable as stated in the following theorem.

Theorem 3.10 ([94]) *Let G be a graph on n vertices and let x be a Perron vector of the distance matrix $\mathcal{D}$ of G. Consider two vertices u and v in G.*

(1) If $N(u) \setminus \{v\} \subsetneq N(v) \setminus \{u\}$, then $x_u > x_v$.
(2) If $N(u) \setminus \{v\} = N(v) \setminus \{u\}$, then $x_u = x_v$.

Note that *(2)* of Theorem 3.10 was also proved in [98].

Das [45] investigated the problem of finding upper and lower bounds on the minimal and maximal entries of the Perron vector of distance matrix. The results of these investigations [45] are gathered in the next theorem. First, we need the following definition. The independence number of a graph G, denoted by $\alpha = \alpha(G)$, is the size of a maximum independent set (a set of pairwise non–adjacent vertices) of G. A *complete split graph* with parameters n, q $(q \leq n)$, denoted by $CS(n, q)$, is a graph on n vertices consisting of a clique (a set of pairwise adjacent vertices) on q vertices and an independent set on the remaining $n - q$ vertices in which each vertex of the clique is adjacent to each vertex of the independent set.

Theorem 3.11 ([45]) *Let G be a graph on n vertices with p–norm normalized principal eigenvector $x = (x_1, x_2, \ldots x_n)^T$. Assume that the vertices of G indexed such that $x_1 \geq x_2 \geq \cdots \geq x_n$. Let α, D, δ and S denote the independence number, the diameter, the minimum degree and the sum of the squares of the distances between all unordered pairs of vertices of G. Then*

$$x_n \leq \min\left\{\left(\frac{(\partial_1 - n + \alpha + 1)^p}{(n-\alpha)\alpha^p + \alpha(\partial_1 - n + \alpha + 1)^p}\right)^{\frac{1}{p}}, \left(\frac{(\partial_1 - 2\alpha + 2)^p}{(n-\alpha)(\partial_1 - 2\alpha + 2)^p + \alpha(n-\alpha)^p}\right)^{\frac{1}{p}}\right\}$$

with equality if and only if G is the complete split graph $CS(n, n-\alpha)$;

$$\begin{aligned} x_n \quad \leq \min \quad & \left\{\left(\frac{\left(\sqrt{\frac{2(n-1)S}{n}} - n + \alpha + 1\right)^p}{(n-\alpha)\alpha^p + \alpha\left(\sqrt{\frac{2(n-1)S}{n}} - n + \alpha + 1\right)^p}\right)^{\frac{1}{p}}, \right. \\ & \left. \left(\frac{\left(\sqrt{\frac{2(n-1)S}{n}} - 2\alpha + 2\right)^p}{(n-\alpha)\left(\sqrt{\frac{2(n-1)S}{n}} - 2\alpha + 2\right)^p + \alpha(n-\alpha)^p}\right)^{\frac{1}{p}}\right\} \end{aligned}$$

with equality if and only if G is the complete graph K_n;

$$\left(\frac{\partial_1^{p-2}}{\partial_1^{p-2} + ((n-1)D - (D-1)\delta)^{p-1}}\right)^{\frac{1}{p}} \leq x_1 \leq \left(\frac{D(\partial_1 - n + 2)^{p-1}}{\partial_1 + D(\partial_1 - n + 2)^{p-1}}\right)^{\frac{1}{p}}$$

with equality at both bounds if and only if G is the complete graph K_n;

$$\left(\frac{(n-1)^{p-2}}{(n-1)^{p-2} + ((n-1)D - (D-1)\delta)^{p-1}}\right)^{\frac{1}{p}} \leq x_1 \leq \left(\frac{D\left(\sqrt{\frac{2(n-1)S}{n}} - n + 2\right)^{p-1}}{\sqrt{\frac{2(n-1)S}{n}} + D\left(\sqrt{\frac{2(n-1)S}{n}} - n + 2\right)^{p-1}}\right)^{\frac{1}{p}}$$

with equality at both bounds if and only if G is the complete graph K_n.

A *comet*, also called a *broom*, $CO_{n,\Delta}$ is the tree obtained from a star $S_{\Delta+1}$ and a path $P_{n-\Delta}$ by the coalescence of an endpoint of $P_{n-\Delta}$ with a pendent vertex of $S_{\Delta+1}$. A *double comet*, also called a *double broom* and *dumbbell*, DC_{n,Δ_1,Δ_2} is the tree obtained from a path $P_{n-\Delta_1-\Delta_2+2}$ by attaching $\Delta_1 - 1$ pendent vertices to one endpoint of the path and $\Delta_2 - 1$ pendent vertices to the other endpoint.

In order to characterize the graphs maximizing the distance spectral radius over the class of graphs with given matching number (see Theorem 5.50), Nath and Paul [102] proved a series of results about the components of the distance Perron vector of a double comet.

Theorem 3.12 ([102]) *Let $G = DC_{n,k+t+1,k+1}$ be a double comet of diameter $D = 2d$ and $v_0v_1 \cdots v_{2d}$ a diametrical path in it, where $t \geq 0$. If $X = (\underbrace{x_0, \ldots x_0}_{k}, x_1, x_2, \ldots, x_{2d-1}, \underbrace{x_{2d}, \ldots x_{2d}}_{k+t})^T$ is the distance Perron vector of G, then $x_{d-i} \geq x_{d+i}$, for $1 \leq i \leq d$, with equality if and only if $t = 0$. Moreover, if $t \geq 1$, then $(x_{d-i} - x_{d+i}) > (x_{d-i+1} - x_{d+i-1})$, for $1 \leq i \leq d-1$, and $(x_0 - x_{2d})(\partial_1(G) + 2) = (x_1 - x_{2d-1})\partial_1(G)$.*

Theorem 3.13 ([102]) *Let $G = DC_{n,k+t+1,k+1}$ be a double comet of diameter $D = 2d+1$ and $v_0v_1 \cdots v_{2d+1}$ a diametrical path in it, where $t \geq 0$. If $X = (\underbrace{x_0, \ldots x_0}_{k}, x_1, x_2, \ldots, x_{2d}, \underbrace{x_{2d+1}, \ldots x_{2d+1}}_{k+t})^T$ is the distance Perron vector of G, then $x_{d-i} \geq x_{d+i+1}$, for $1 \leq i \leq d$, with equality if and only if $t = 0$. Moreover, if $t \geq 1$, then $(x_{d-i} - x_{d+i+1}) > (x_{d-i+1} - x_{d+i})$, for $1 \leq i \leq d-1$, and $(x_0 - x_{2d+1})(\partial_1(G) + 2) = (x_1 - x_{2d})\partial_1(G)$.*

The above two theorems were generalized by Wang and Zhou [138] to the class of all graphs as follows.

Theorem 3.14 ([138]) *Let u and v be two vertices in a graph G. Let u' and v' be two pendent neighbors of u and v, respectively. Then $(\partial_1(G) + 2)(x_{v'} - x_{u'}) = \partial_1(G)(x_v - x_u)$, where x_w denote the component of the distance Perron vector corresponding the vertex w.*

4 Transformations, operations and particular Spectra

In this section, we give the distance spectra of some particular families of graphs. We also give an overview of the results about the distance spectrum of a graph obtained by means of some transformations from another graph. Of course, the distance spectrum of the new graph is given in function of that of the original graph. Similar overview is furnished for the graphs obtained using operations involving two graphs. Note that the results are stated as theorems, but most of them were originally stated as lemmas.

First, since the diagonal entries of the distance matrix are all 0, the distance spectrum of any graph contains at least two distinct eigenvalues. Indulal [82] showed that K_n is the only graph that contains exactly two distinct distances eigenvalues. The distance matrix of the complete graph coincides with its adjacency matrix, and therefore, the distance spectrum of K_n equals its adjacency spectrum.

Hosoya, Murakami and Gotoh [74] calculated the distance characteristic polynomial for a path P_n:

$$P_{\mathcal{D}(P_n)}(t) = (-1)^n t^n + (-1)^{(n-1)} \sum_{k=2}^{n} 2^{(k-2)}(k-1)\frac{n^2(n^2-1)(n^2-2)\cdots(n^2-(k-1)^2)}{k^2(k^2-1)(k^2-2^2)\cdots(k-(k-1)^2)} t^{(n-k)}.$$

Hosoya, Murakami and Gotoh [74] computed the distance characteristic polynomial for the even cycles and Graovac [66] did it for both odd and even cycles (see also [58]):

If $n = 2p$ (*i.e., even*)

$$P_{\mathcal{D}(C_n)}(t) = t^{p-1} \cdot \left(t - \frac{n^2}{4}\right) \cdot \prod_{j=1}^{p} \left(t + \csc^2\left(\frac{\pi(2j-1)}{n}\right)\right).$$

If $n = 2p+1$ (*i.e., odd*)

$$P_{\mathcal{D}(C_n)}(t) = \left(t - \frac{n^2-1}{4}\right) \cdot \prod_{j=1}^{p} \left(t + \frac{1}{4}\sec^2\left(\frac{\pi j}{n}\right)\right) \cdot \prod_{j=1}^{p} \left(t + \frac{1}{4}\csc^2\left(\frac{\pi(2j-1)}{2n}\right)\right).$$

Caporossi, Chasset and Furtula [32] computed partially the distance spectrum of a multipartite graph.

Theorem 4.1 ([32]) *For the complete multipartite graph $K_{n_1,\ldots,n_k}$, let $m_j = |\{i : n_i = j\}|$, $j \geq 1$. Whenever $m_j \geq 2$, the distance spectrum of $K_{n_1,\ldots,n_k}$ contains the eigenvalue $j-2$ with multiplicity at least $m_j - 1$, and eigenvalue -2 with multiplicity at least $\sum_{i\geq 2} m_j(j-1)$.*

The cocktail party graph CP_p on $n = 2p$ vertices can be considered as a p–partite graph $K_{2,\ldots,2}$. Then, as a consequence of Theorem 4.1, the eigenvalues of CP_p are $2p$, 0 with multiplicity $p-1$, and -2 with multiplicity p.

Collins [36] computed the distance characteristic polynomial of the star S_n on n vertices:

$$P_{\mathcal{D}(S_n)}(t) = (-1)^{n-1}\left(t^2 - 2(n-2)t - n + 1\right)(t+2)^{n-2}.$$

A *double star* S_{Δ_1,Δ_2} is the tree obtained from a K_2 by attaching $\Delta_1 - 1$ pendent vertices to one vertex and $\Delta_2 - 1$ pendent vertices to the other vertex (see Figure 19 for the double star $S_{6,4}$). The double star S_{Δ_1,Δ_2} contains $n = \Delta_1 + \Delta_2$ vertices among which $n-2$ are pendent, and the two non pendent vertices have degrees Δ_1 and Δ_2 respectively. The distance characteristic polynomial of the double star $S_{\Delta,\Delta}$ on $n = 2\Delta$ vertices was computed by Collins [36]:

$$P_{\mathcal{D}(S_{\Delta,\Delta})}(t) = (t+n)(t+1)\left(t^2 - (5n-1)t - 9n\right)(t+2)^{2\Delta-4}.$$

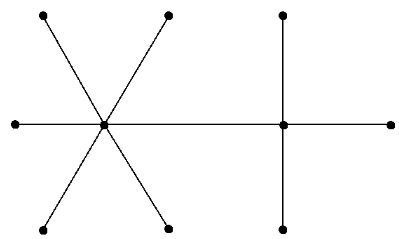

Figure 19: The double star $S_{6,4}$.

The *full k–ary tree* of length r, denoted $F_{r,k}$, is defined recursively by: $F_{1,k}$ is the star S_{k+1} on $k+1$ vertices, and $F_{r,k}$ is obtained from $F_{r-1,k}$ by attaching k new edges to each pendent vertex (see Figure 20 for $F_{2,4}$). Collins [36] computed the distance characteristic polynomial of the full k–ary tree to be

$$P_{F_{r,k}}(t) = Q_{r+1,k}(t) \cdot \prod_{i=1}^{k} R_{i,k}^{(k-1)k^{k-i}}(t),$$

where $Q_{r+1,k}(t)$ is the polynomial of degree $r+1$, defined by

$$Q_{1,k}(t) = -t \quad \text{and} \quad \sum_{p=1}^{\infty} Q_{p,k}(t)x^p = \frac{N(k,t,x)}{M(k,t,x)}$$

with
$N(k,t,x) = -(ktx)^5 + k^3t^3x^4((3k+1)t + (2k+2)) + k^2tx^3((3k+3)t^2 + (2k+6)t + 3) + kx^2((k+3)t^2 + 4t + 1) + tx$,
$M(k,t,x) = (ktx+1)(kt^2x^2 + x(2+(k+1)t) + 1) \cdot (k^3t^2x^2 + kx(2+(k+1)t) + 1)$,
and the polynomials $R_{i,k}(t)$ are defined recursively by
$R_{0,k}(t) = 1$; $R_{1,k}(t) = -t-2$; $R_{i+1,k}(t) = -((k+1)t+2)R_{i,k}(t) - kt^2R_{i-1,k}(t)$.

The distance matrix of a graph G with diameter 2 can be written in terms of the adjacency matrices of G and its complement $\overline{G}$: $\mathcal{D} = A + 2\overline{A}$. Such a relationship does not exist between the spectra of $\mathcal{D}$, A and $\overline{A}$ in general. However, if in addition to have a diameter 2, G is regular, the distance spectrum of G can be obtained from its adjacency spectrum as stated in the next theorem.

Theorem 4.2 ([56, 85]) *Let G be a k–regular graph on n vertices with diameter at most 2 and adjacency spectrum $\lambda_1 = k, \lambda_2, \lambda_3, \ldots, \lambda_n$. Then the distance spectrum of G is $2n-2-k, -(2+\lambda_2), -(2+\lambda_3), \ldots, -(2+\lambda_n)$.*

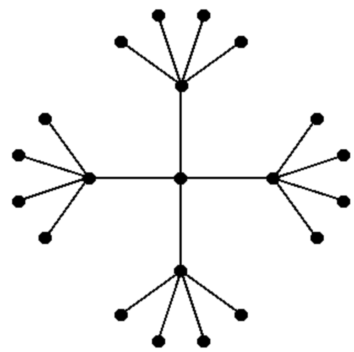

Figure 20: The full 4–ary tree of length 2: $F_{2,4}$.

An $n \times n$–matrix C is *circulant* [47] if it takes the following form:

$$C = \begin{bmatrix} C_1 & C_n & C_{n-1} & \dots & C_3 & C_2 \\ C_2 & C_1 & C_n & \dots & C_4 & C_3 \\ C_3 & C_2 & C_1 & \dots & C_5 & C_4 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ C_{n-1} & C_{n-2} & C_{n-3} & \dots & C_1 & C_n \\ C_n & C_{n-1} & C_{n-2} & \dots & C_2 & C_1 \end{bmatrix}.$$

A graph is called *circulant* if its adjacency matrix is circulant. A graph is called integral if all eigenvalues of its adjacency matrix are integers. For more about integral graphs see [12] as well as the references therein. An *integral circulant* graph is a circulant graph with an integral adjacency spectrum (see *e.g.* [127]). Let Div be a set of positive, proper divisors of the integer $n \geq 1$. Define the graph $ICG_n(Div)$ to have vertex set $V = \{0, 1, \dots, n-1\}$ and edge set $E = \{\{a, b\} \mid a, b \in V, \ \gcd(a-b, n) \in Div\}$. In the particular case $Div = \{1\}$, the graph $ICG_n(1)$ is called the *unitary Cayley graph*. Figure 21 illustrates the unitary Cayley graph $ICG_{10}(1)$. Its distance spectrum is $(15, 1, 0, 0, 0, 0, -4, -4, -4, -4)$.

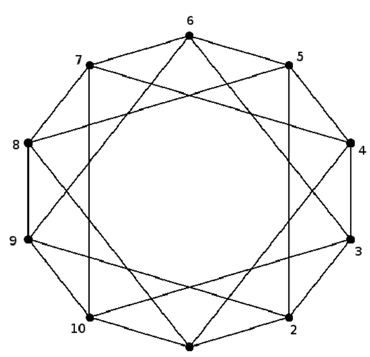

Figure 21: The unitary Cayley graph $ICG_{10}(1)$.

Ilić [78] proved that the distance eigenvalues of an integral circulant graph are integers.

Theorem 4.3 ([78]) *An integral circulant graph $ICG_n(Div)$, where Div is an arbitrary set of divisors of n, has integral distance spectra.*

Ilić [78] also calculated the spectrum of the unitary Cayley graph $ICG_n(1)$ on n vertices according to the values of n.

- If n is a prime, then $ICG_n(1)$ is the complete graph K_n and therefore its distance spectrum is its adjacency spectrum: $\partial_1 = n-1$ and $\partial_2 = \cdots = \partial_n = -1$.
- If n is a power of 2, then $ICG_n(1)$ is the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ and its distance spectrum is $\partial_1 = \frac{3n}{2} - 2$, $\partial_2 = \frac{n}{2} - 2$ and $\partial_3 = \cdots = \partial_n = -2$.
- If n is odd composite number, then the distance spectrum of $ICG_n(1)$ is $\partial_1 = 2(n-1) - k$ and $\partial_i = -2 - c(i-1,n)$, for $i = 2,\ldots,n$, where k denotes the degree of any vertex in (the regular) graph $ICG_n(1)$, and

$$c(r,n) = \sum_{\substack{a=1 \\ \gcd(a,n)=1}}^{n} \omega_n^{a\cdot r}$$

  and where ω_n denotes a complex primitive nth root of unity.
- If n is even with an odd prime divisor, using the same notation as the previous case, the distance spectrum of $ICG_n(1)$ is $\partial_1 = \frac{5n}{2} - 2(k+1)$, $\partial_2 = 2(k-1) - \frac{n}{2}$, $\partial_i = -2 - c(i-2,n)$, for $i = 2,\ldots,\frac{n}{2}+1$, and $\partial_i = -2 - c(i-1,n)$, for $i = \frac{n}{2}+2,\ldots,n$.

Some families of graphs are defined using operations on other graphs. We next give descriptions of distance spectra of graphs obtained using operations, involving two graphs or more. We give the distance spectra of certain families.

Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Take another copy of G with set of vertices $\{u_1, u_2, \ldots, u_n\}$ labelled such that u_i corresponds to v_i for each i. Make u_i adjacent to all the vertices in $N(v_i)$ in G, for each i. The resulting graph, denoted by D_2G, is called the *double graph* of G (see Figure 22 for the double graph of the cycle C_5). The distance spectrum of the double graph of G was derived from the distance spectrum of G by Indulal and Gutman [84].

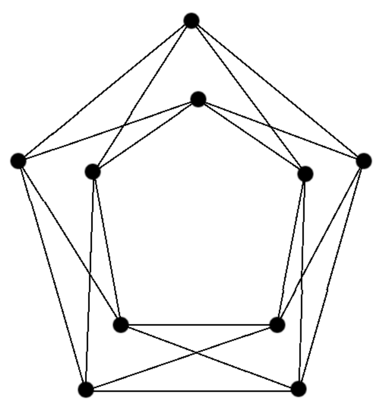

Figure 22: The double graph of the cycle C_5: D_2C_5.

Theorem 4.4 ([84]) *Let G be a graph on n vertices with distance spectrum $\{\partial_1, \partial_2, \ldots, \partial_n\}$. Then the distance eigenvalues of D_2G are $2\partial_1+2, 2\partial_2+2, \ldots, 2\partial_n+2$, and -2 with multiplicity n.*

The distance spectrum of the Cartesian product $G_1 \square G_2$ of two transmission regular graphs G_1 and G_2 was derived from the distance spectra of G_1 and G_2 by Indulal [81].

Theorem 4.5 ([81]) *Let G_1 and G_2 be two transmission regular graphs on n_1 and n_2 vertices with transmission regularity k_1 and k_2 respectively. Let $(k_1, \partial_1^1, \partial_2^1, \ldots, \partial_{n_1}^1)$ and $(k_1, \partial_1^2, \partial_2^2, \ldots, \partial_{n_2}^2)$ be the distance spectra of G_1 and G_2, respectively. Then the distance spectrum of $G_1 \square G_2$ is $\{n_1k_2 + n_2k_1, n_1\partial_i^2, n_2\partial_j^1, 0\}$, where $i = 2,\ldots,n_1$, $j = 2,\ldots,n_2$ and 0 is with multiplicity $(n_1-1)(n_2-1)$.*

Note that Indulal and Gutman [84] proved the above theorem in the particular case where $G_2 \cong K_2$. The next result proved Caporossi, Chasset and Furtula [32] can also be obtained as a corollary of the above theorem, since the graph for which the result is stated can be considered as the Cartesian product of a clique on k vertices and K_2.

Corollary 4.6 ([32]) *Let G be a graph made of two k–cliques connected in such a way that each vertex of a clique is connected to exactly one vertex of the other, then the distance spectrum of G consists of $3k-2$, $-k$, 0 with multiplicity $k-1$, and -2 with multiplicity $k-1$.*

Using Theorem 4.5, Indulal [81] computed the distance eigenvalues of the Hamming graph $H(D,p)$ which are $D(p-1)p^{D-1}, 0$ and $-p^{D-1}$ with multiplicities 1, $p^D - D(p-1) - 1$ and $D(p-1)$ respectively. Another well–known graph defined using the Cartesian product of two cycles is the *nanotorus* $C_k \Box C_m$. To illustrate, the nanotorus $C_3 \Box C_4$ is given in Figure 23. The distance eigenvalues of the nanotorus $C_k \Box C_m$ were computed, also as a consequence of Theorem 4.5, by Indulal [81] when k and m are odd:

$$\frac{(m+k)(mk-1)}{4}, \quad -\frac{m}{4}sec^2\left(\frac{\pi j}{2k}\right), \quad -\frac{m}{4}cosec^2\left(\frac{\pi r}{2k}\right), \quad -\frac{k}{4}sec^2\left(\frac{\pi t}{2m}\right), \quad -\frac{k}{4}cosec^2\left(\frac{\pi l}{2m}\right),$$

where $j \in \{1, 2, \ldots, k-1\}$ and even, $r \in \{1, 2, \ldots, k-1\}$ and odd, $t \in \{1, 2, \ldots, m-1\}$ and even, $l \in \{1, 2, \ldots, m-1\}$ and odd, together with 0 of multiplicity $(m-1)(k-1)$.

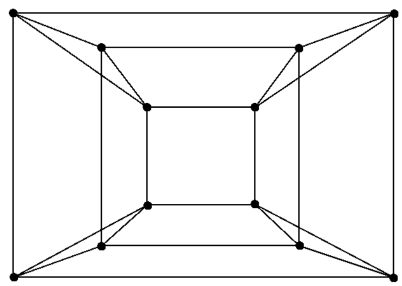

Figure 23: The nanotorus $C_3 \Box C_4$.

The *lexicographic product* or *graph composition* $G \circ H$ of two graphs G and H is the graph whose vertex set is the (set) Cartesian product $V(G) \times V(H)$, and in which two vertices (u, u') and (v, v') are adjacent if and only if either u is adjacent with v in G or $u = v$ and u' is adjacent with v' in H. Indulal [81] showed that the distance spectrum of $G \circ H$, whenever H is regular, can be deduced from the distance spectrum of G and the adjacency spectrum of H.

Theorem 4.7 ([81]) *Let G and H be two graphs on p and n vertices respectively. Assume that H is k–regular. Let $\{\partial_1, \partial_2, \ldots, \partial_p\}$ and $\{\lambda_1 = k, \lambda_2, \ldots, \lambda_n\}$ be the distance and adjacency spectra of G and H respectively. Then the distance eigenvalues of $G \circ H$ are $n\partial_i + 2n - k - 2$ with multiplicity 1 and $-\lambda_j - 2$ with multiplicity p, for $i = 1, 2, \ldots, p$ and $j = 2, 3, \ldots, n$.*

Note that Indulal and Gutman [84] proved the above theorem in the particular case where $H \cong K_2$.

Let G be a graph. Attach a pendant vertex to each vertex of G. The resulting graph, denoted by $Cor(G)$, is called the *corona of G with K_1* (see Figure 24 for $Cor(C_6)$). Indulal and Gutman [84] computed the distance spectrum of the corona of a transmission regular graph G from its distance spectrum.

Theorem 4.8 ([84]) *Let G be a k–transmission regular graph on n vertices with distance spectrum $\{\partial_1 = k, \partial_2, \ldots, \partial_n\}$. Then the distance spectrum of $Cor(G)$ consists of $\partial_i - 1 + \sqrt{\partial_i^2 + 1}$ and $\partial_i - 1 - \sqrt{\partial_i^2 + 1}$, for $i = 2, 3, \ldots, n$ together with $n + k - 1 - \sqrt{(n+k)^2 + (p-1)^2}$ and $n + k - 1 + \sqrt{(n+k)^2 + (p-1)^2}$.*

To prove the above theorem, Indulal and Gutman [84] first established the next result.

Theorem 4.9 ([84]) *Let $\mathcal{D}$ be the distance matrix of a k–transmission regular graph G on n vertices. Let $\partial_1 = k, \partial_2, \ldots, \partial_n$ be the distinct distance eigenvalues of G. Then $\mathcal{D}$ is irreducible and there exists a polynomial*

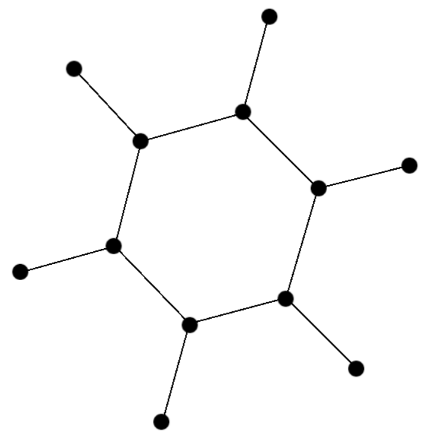

Figure 24: The corona graph of the cycle C_6 with K_1:$Cor(C_6)$.

$P(x)$ such that $P(\mathcal{D}) = J$, where J is the all 1's $n \times n$ matrix. In this case

$$P(x) = \frac{n(x-\partial_2)(x-\partial_3)\cdots(x-\partial_n)}{(k-\partial_2)(k-\partial_3)\cdots(k-\partial_n)}.$$

Let G be a graph on the vertex set $\{v_1, v_2, \ldots, v_n\}$. Define the bipartite graph $EDC(G)$, called *extended double cover graph* of G, with vertex set $\{v_1, v_2, \ldots, v_n, u_1, u_2, \ldots, u_n\}$ in which v_i is adjacent to u_i for each $i = 1, 2, \ldots, n$ and v_i is adjacent to u_j if v_i is adjacent to v_j in G. For instance, the extended double cover graph of the complete graph K_n is the complete bipartite graph $K_{n,n}$. The graph $EDC(C_4)$ is illustrated in Figure 25.

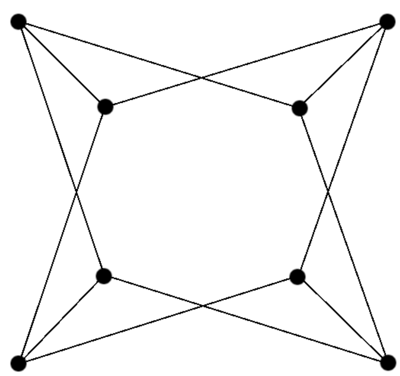

Figure 25: The extende double cover graph of C_4: $EDC(C_4)$.

Indulal and Gutman [84] calculated the distance spectrum of the extended double cover graph of a k–regular graph of diameter 2 from its adjacency spectrum.

Theorem 4.10 ([84]) *Let G be a k–regular graph on n vertices with diameter 2 and adjacency spectrum $\{\lambda_1 = k, \lambda_2, \ldots, \lambda_n\}$. Then the distance eigenvalues of $EDC(G)$ are $5n-2k-4$, $2k-n$, $-2(\lambda_i+2)$, and $2\lambda_i$ for $i = 2, 3, \ldots, n$.*

The *join* $G\nabla H$ of two vertex–disjoint graphs G and H is the graph obtained from the union $G \cup H$ by adding all possible edges between each vertex of G and each vertex of H. Stevanović and Indulal [132] proved that it is possible to deduce the distance spectrum of the join of two regular graphs from their adjacency spectra.

Theorem 4.11 ([132]) *For $i = 1, 2$, let G_i be a k_i–regular graph on n_i vertices with adjacency eigenvalues $\lambda_{i,1} = k_i, \lambda_{i,2}, \ldots, \lambda_{i,n_i}$. The distance spectrum of $G_1 \nabla G_2$ consists of $-\lambda_{i,j_i} - 2$, $i = 1, 2$ and $2 \leq j_i \leq n_i$,* *and two more eigenvalues of the form*

$$n_1 + n_2 - 2 - \frac{k_1 + k_2}{2} \pm \sqrt{\left(n_1 - n_2 - \frac{k_1 - k_2}{2}\right)^2 + n_1 n_2}$$

Stevanović and Indulal [132] computed (as a corollary of Theorem 4.11) the distance eigenvalues of a complete bipartite graph $K_{p,q}$. They are $p + q - 2 \pm \sqrt{p^2 - pq + q^2}$ and -2 with multiplicity $p + q - 2$.

The *wheel graph* W_n on $n \geq 4$ vertices is the join graph of C_{n-1} and K_1 (see Figure 26 for W_{10}).

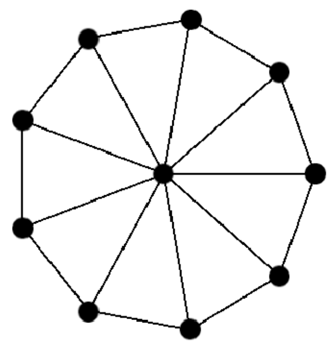

Figure 26: The wheel graph W_{10}.

The distance spectrum of a wheel graph W_n, first calculated in [85], can be deduced from the adjacency eigenvalues of C_{n-1}, say $t_1 = 2 > t_2 \geq \cdots \geq t_{n-1}$, using Theorem 4.11. The distance eigenvalues of W_n are $n - 3 \pm \sqrt{n^2 - 5n + 8}$ and $-t_i - 2$ for $2 \leq i \leq n - 1$.

Also, as a consequence of Theorem 4.11, the distance eigenvalues of the complete split graph $CS(n, q) = K_q \nabla \overline{K}_{n-q}$ are -1 with multiplicity $q - 1$, -2 with multiplicity $n - q - 1$ and

$$n - \frac{q + 3}{2} \pm \sqrt{\frac{(n - 3q + 1)^2}{4} + q(n - q)}.$$

Note that a particular case of Theorem 4.11, namely the distance characteristic polynomial of the join of two graphs of diameter at most 2, was provided by Ramane, Gutman and Revankar [109].

Concerning the join of a graph with the union of two graphs Stevanović and Indulal [132] proved the next theorem.

Theorem 4.12 ([132]) *For $i = 0, 1, 2$ let G_i be a k_i–regular graph on n_i vertices with adjacency eigenvalues $\lambda_{i,1} = k_i \geq \lambda_{i,2}, \ldots, \lambda_{i,n_i}$. If $k_1 \neq k_2$, the distance spectrum of $G_0 \nabla (G_1 \cup G_2)$ consists of $-\lambda_{i,j_i} - 2$, $i = 0, 1, 2$ and $2 \leq j_i \leq n_i$, and three more eigenvalues which are solutions of the cubic equation in t*

$$(2n_0 - k_0 - 2 - t)(t + k_1 + 2)(t + k_2 + 2) + (2(t + k_0 + 2) - 3n_0)(n_1(t + k_2 + 2) + n_2(t + t_1 + 2)) = 0.$$

Stevanović [129] generalized the notion of join of graphs to that of *joined union* of graphs as follows. Let $G = (V, E)$ be a graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$, and for $i = 1, 2, \ldots, n$, let $G_i = (V_i, E_i)$ be a graph of order n_i. The *joined union* graph of $G_1, G_2, \ldots, G_n$ with respect to G, denoted $G[G_1, G_2, \ldots, G_n]$, is the graph whose vertex set W and edge set F are

$$W = \bigcup_{i=1}^{n} V_i \quad \text{and} \quad F = \left(\bigcup_{i=1}^{n} E_i\right) \bigcup \left(\bigcup_{v_i v_j \in E} V_i \times V_j\right).$$

Theorem 4.13 ([129]) *Let G be a graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$, and for $i = 1, 2, \ldots, n$, let G_i be a k_i–regular graph on n_i with adjacency eigenvalues $\lambda_{i,1} = k_i \geq \lambda_{i,2} \geq \ldots \geq \lambda_{i,n_i}$. The distance spectrum of the joined union $G[G_1, G_2, \ldots, G_n]$ consists of the eigenvalues $-\lambda_{i,j} - 2$ for $i = 1, 2, \ldots, n$ and $j = 2, 3, \ldots, n_i$ and the eigenvalues of the matrix*

$$\begin{bmatrix} 2n_1 - k_1 - 2 & d(v_1, v_2)n_2 & d(v_1, v_3)n_3 & \ldots & d(v_1, v_n)n_n \\ d(v_2, v_1)n_1 & 2n_2 - k_2 - 2 & d(v_2, v_3)n_3 & \ldots & . \\ d(v_3, v_1)n_1 & d(v_3, v_2)n_2 & 2n_3 - k_3 - 2 & \ldots & . \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ d(v_n, v_1)n_1 & d(v_n, v_2)n_2 & d(v_n, v_3)n_3 & \ldots & 2n_n - k_n - 2 \end{bmatrix}.$$

A graph G is said to be *self–complementary* if $G \cong \overline{G}$, where $\overline{G}$ denotes the complement of G. For a given graph G, consider the graph $P_4(G)$ obtained from a path P_4 by replacing each of its endpoints by a copy of G, and each of its internal vertices by a copy of $\overline{G}$, and then joining the vertices of these graphs by all possible edges whenever the corresponding vertices of P_4 are adjacent (see Figure 27 for $P_4(K_3)$). The graph $P_4(G)$ is a self–complementary graph.

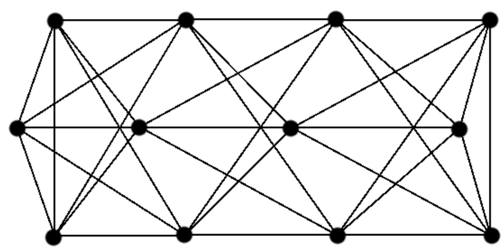

Figure 27: The self–complementary grap $P_4(K_3)$.

Theorem 4.14 ([83]) *Let G be a k–regular graph on n vertices, with adjacency spectrum $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$. Then the distance spectrum of $P_4(G)$ consists of $-\lambda_i - 2$ and $\lambda_i - 1$, for $i = 2, 3, \ldots, n$, each with multiplicity 2, together with*

$$\frac{7n - 3 \pm \sqrt{(2k+1)^2 + 45n^2 - 12nk - 6n}}{2} \quad \textit{and} \quad \frac{n + 3 \pm \sqrt{(2k+1)^2 + 5n^2 + 4nk + 2n}}{2}.$$

Now, we turn to the description of the behavior of the distance spectral radius of a graph when some transformations are performed within the graph itself. We begin with the transformation consisting of deletion or addition of an edge.

Let $e = uv$ be an edge of a graph G such that $G' = G - e$ is connected. The removal of e increases some distances and does not change some others, thus by the Perron–Frobenius theorem, one can conclude that $\partial_1(G) < \partial_1(G')$. In particular, for any spanning tree T of G, we have that $\partial_1(T) \geq \partial_1(G)$ with equality if and only if G is a tree, *i.e.*, $T = G$. Similarly, adding a new edge to G decreases the distance spectral radius. As immediate consequences of that fact,

- the complete graph K_n minimizes the distance spectral radius among all graphs of order n;
- the complete bipartite graph $K_{p,q}$ minimizes the distance spectral radius among all bipartite graphs with a partition into two sets of p and q vertices respectively.

Let u, v and w three vertices in a graph $G = (V, V)$ such that $uv \in E$ and $uw \notin E$. The *rotation* of the edge uv to uw is the operation that consists of the deletion of uv and then the addition of uw. Under certain conditions, the rotation of a pendent edge increases the distance spectral radius.

Stevanović and Ilić [131] used Theorem 3.6 and Theorem 3.7 to prove the next result, stated using the notations of those theorems.

Theorem 4.15 ([131]) *Let G be a graph and v one of its vertices. If $k \geq l \geq 1$, then*

$$\partial_1(G(v,k,l)) < \partial_1(G(v,k+1,l-1)).$$

Ning, Ouyang and Lu [105] used the above result to prove the next one.

Theorem 4.16 ([105]) *If a tree T minimizes the distance spectral radius over the set of all trees of order n with r pendent vertices, the lengths of any two adjacent pendent paths in T are almost the same.*

Zhang and Godsil [149] showed that Theorem 4.15 remains true if the vertex v is replaced by an edge, *i.e.*, two paths are attached to two adjacent vertices instead of to the same vertex.

Theorem 4.17 ([149]) *Let u and v be two adjacent vertices of a graph G and for positive integers k and l, let $G_{k,l}$ denote the graph obtained from G by adding paths of length k at u and length l at v. If $k > l \geq 1$, then $\partial_1(G_{k,l}) < \partial_1(G_{k+1,l-1})$; if $k = l \geq 1$, then $\partial_1(G_{k,l}) < \partial_1(G_{k+1,l-1})$ or $\partial_1(G_{k,l}) < \partial_1(G_{k-1,l+1})$.*

Instead of the rotation of an endedge of an appended path to an endedge of another appendent path, Bose, Nath and Paul [22] considered the rotation of a pendent edge belonging to a set of pendent edges with a common neighbor to another similar edge. They get the following result.

Theorem 4.18 ([22]) *Let G be a graph with a clique K_s of order $s \geq 2$ and u, v be two vertices on the clique with p, q pendent vertices, respectively, where $d(v) = q + s - 1$ in G. If $G' = G - vw + uw$ (see Figure 28), where w is a pendent vertex adjacent to v in G then for $p \geq q \geq 1$, $\partial_1(G) > \partial_1(G')$.*

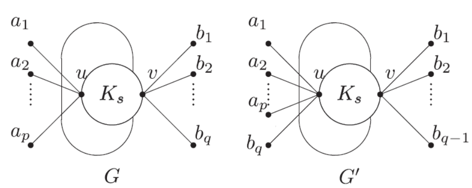

Figure 28: The graphs G and G' in Theorem 4.18.

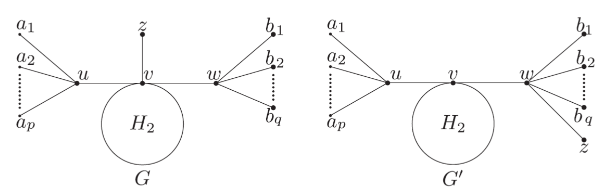

Figure 29: The graphs G and G' in Theorem 4.19.

Bose, Nath and Paul [22] proved a result similar to that of Theorem 4.18 for a particular rotation.

Theorem 4.19 ([22]) *Let H_1 be a path $P \cong uvw$ with p and q $(p \geq q)$ pendent vertices adjacent to u and w, respectively, one pendent vertex z adjacent to v, and H_2 is any graph. If G is a graph obtained by identifying the vertex v with any vertex of H_2 and $G' = G - vz + wz$ (see Figure 29), then $\partial_1(G') > \partial_1(G)$.*

Theorem 4.20 ([21]) *If G' is the graph obtained from G by the rotation of the edge v_1v_2 to v_1v_4 as illustrated in Figure 30, then $\partial_1(G) > \partial_1(G')$.*

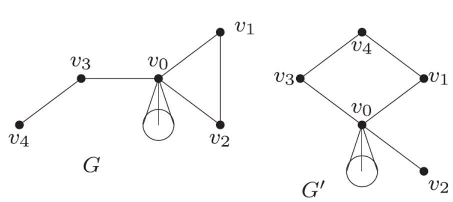

Figure 30: The graphs G and G' of Theorem 4.20.

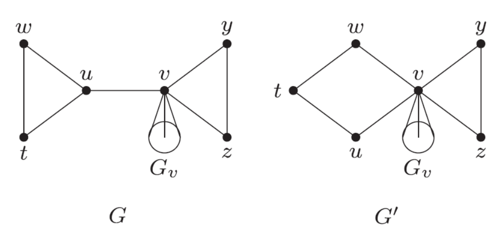

Figure 31: The graphs G and G' of Theorem 4.22.

Theorem 4.21 ([21]) *Let $v_1v_2v_3\cdots v_gv_1$ be a chain in a graph G of length at least 4. For $1 \leq i \leq g$, let G_i be the graph attached at v_i, and S_i be the sum of the components of the Perron vector of G corresponding to the vertices in G_i. If $S_1 = \max\{S_j | 1 \leq j \leq g\}$ and $G' = G - v_1v_g + v_gv_{g-2}$, then $\partial_1(G') > \partial_1(G)$.*

Theorem 4.22 ([21]) *If G and G' are the graphs as shown in Figure 31, then $\partial_1(G) > \partial_1(G')$.*

Another particular case of an rotation is considered by Wang and Zhou [138] in the next theorem.

Theorem 4.23 ([138]) *Consider a comet $CO_{n,n-2d+1}$ with an odd diameter $2d+1$ whose vertices are labeled as in Figure 32. Let G be the graph obtained form $CO_{n,n-2d+1}$ by the coalescence of the central vertex of its diametrical path with a vertex of a nontrivial connected graph H (see Figure 4.23. Let $G' = G - u_{d-1}u_d + v_{d-1}u_d$. Then $\partial_1(G') < \partial_1(G)$.*

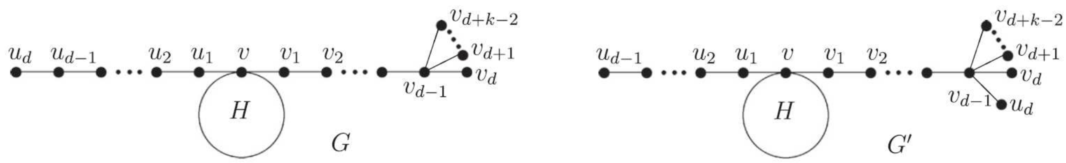

Figure 32: The graphs G and G' im Theorem 4.23.

A natural generalization of the rotation of an edge is the rotation of two or more edges incident with the same vertex to edges incident to another vertex. The behavior of the spectral distance radius under this generalized rotation subjected to additional conditions was also studied. We begin by the particular case proved by Zhang and Godsil [149].

Theorem 4.24 ([149]) *Let C_1 be a component of $G-u$ and $v_1,\ldots,v_k$, with $1 \le k \le d_G(u) - d_{C_1}(u)$, be some vertices of $N_G(u) \setminus N_{C_1}(u)$. Suppose $N_{C_1}(u) \setminus \{v\} = N_{C_1}(v)$, where v is a vertex of C_1 adjacent to u. Let G' be the graph obtained from G by deleting the edges uv_s and adding the edges vv_s ($1 \le s \le k$). If there exists a vertex $w \in V(G) \setminus (V(C_1) \cup \{u\})$ such that $d_G(w, v_s) < d_{G'}(w, v_s)$, for all $1 \le s \le k$, then $\partial_1(G) < \partial_1(G')$.*

Bose, Nath and Paul [21] generalized Theorem 4.18, which is their own theorem but in another paper [22], to the next one. The generalization consists in replacing the pendent edge attached to a vertex belonging to a clique by a subgraph attached to a vertex, also belonging to the clique.

Theorem 4.25 ([21]) *Let G be a graph on n vertices with a clique K_s such that $G - E(Ks)$ has exactly s components of which at least two, say G_1 and G_2, are not trivial. Let $u \in V(K_s) \cap V(G_1)$ and $v \in V(K_s) \cap V(G_2)$. If $G' = G - \{vw, w \in N_{G_2}(v)\} + \{uw, w \in N_{G_2}(v)\}$, then $\partial_1(G) > \partial_1(G')$.*

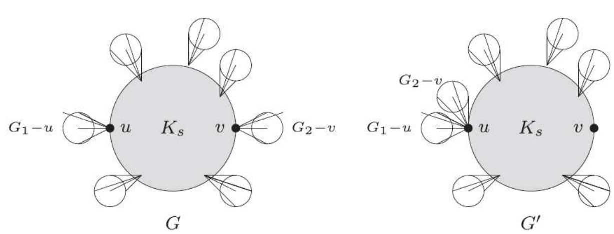

Figure 33: The graphs G and G' of Theorem 4.25.

The above theorem can also be seen as a generalization of the next two results.

Theorem 4.26 ([21]) *If G and G' are the graphs as shown in Figure 34, where both G_u and G_v are non trivial graphs and G_v has at least three vertices, then $\partial_1(G) > \partial_1(G')$.*

Theorem 4.27 ([21]) *If G and G' are the graphs as shown in Figure 35, where G_1 is non trivial, then $\partial_1(G) > \partial_1(G')$.*

The next three theorems are stated on the behavior of the distance spectral radius under rotation of a set of edges, all incident with the same vertex, under conditions on the components of the Perron vector.

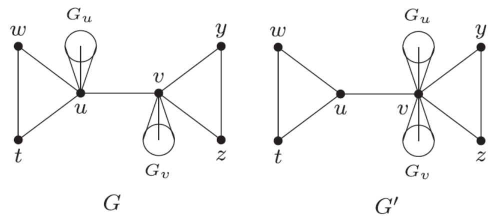

Figure 34: The graphs G and G' of Theorem 4.26.

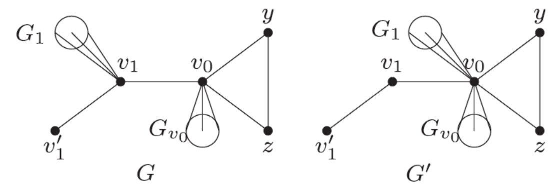

Figure 35: The graphs G and G' of Theorem 4.27.

Theorem 4.28 ([143]) *Suppose the graph* $G = \cup_{i=1}^{3} G_i$ *satisfies that* $G_i \cap G_j = \{v_0\}$ *for* $1 \le i, j \le 3$, $i \ne j$, *and that* $|V(G_i)| \ge 2$ *for* $i = 1, 2, 3$ *(see Figure 36 (a)). Let* $X = (x_0, x_1, \ldots, x_{n-1})^T$ *be the Perron eigenvector corresponding to* $\partial_1(G)$, *in which* x_i *corresponds to* v_i. *Let*

$$S_1 = \sum_{v_i \in V(G_1)} x_i, \qquad S_2 = \sum_{v_i \in V(G_2)} x_i$$

and for a vertex $v_a \in V(G_2)$, $v_a \ne v_0$, *let* $H = G - \{v_0 v_i, v_i \in N_{G_3}(v_0)\} + \{v_a v_i, v_i \in N_{G_3}(v_0)\}$. *If* $S_1 \ge S_2$, *then* $\partial_1(H) > \partial_1(G)$.

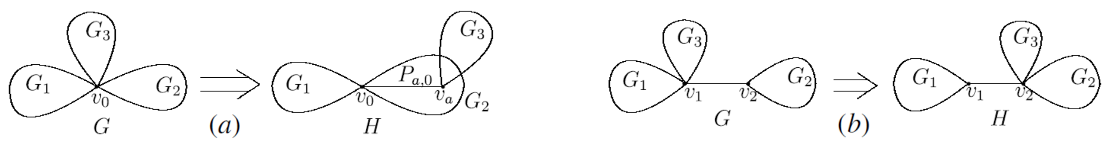

Figure 36: Transformations in Theorem 4.28 and Theorem 4.29.

Theorem 4.29 ([143]) *Assume that the graph* G *shown in Figure 36 (b) satisfies* $G_1 \cap G_3 = \{v_1\}$ *and* $v_1 v_2$ *is a cut edge. Let* $X = (x_0, x_1, \ldots, x_{n-1})^T$ *be the Perron eigenvector corresponding to* $\partial_1(G)$, *in which* x_i *corresponds to* v_i. *Let*

$$S_1 = \sum_{v_i \in V(G_1)} x_i, \qquad S_2 = \sum_{v_i \in V(G_2)} x_i,$$

and let $H = G - \{v_1 v_i, v_i \in N_{G_3}(v_1)\} + \{v_2 v_i, v_i \in N_{G_3}(v_1)\}$. *If* $S_1 \ge S_2$ *and* $|V(G_3)| \ge 2$, *then* $\partial_1(H) > \partial_1(G)$.

In [144], Yu, Wu and Shu considered the rotation of the edges incident to the same vertex and satisfying a given condition.

Theorem 4.30 ([144]) *Let* G *be a graph such that* $G = G_p \cup G_0 \cup G'$ *with* $G_p \cap G_0 = G_p \cap G' = G_0 \cap G' = \{v_0\}$ *and* G_p *consisting of pendent edges* $v_0v_1, v_0v_2, \ldots, v_0v_k$ $(k \ge 4)$. *Let* $S' = V(G')$ *and suppose that* $N_{G'}(v_0) = N_1 \cup N_2$ *satisfying that* $N1 \ne \emptyset$, $N_2 \ne \emptyset$, $N_1 \cap N_2 = \emptyset$. *Let*

$$H = G - \sum_{v_i \in N_1} v_i v_0 + \sum_{v_i \in N_1} v_i v_k \qquad \textit{or} \qquad H = G - \sum_{v_i \in N_2} v_i v_0 + \sum_{v_i \in N_2} v_i v_k.$$

For any vertex $v_j \in S' \setminus \{v_0\}$, *if all paths from* v_0 *to* v_j *with a length of* $d_G(v_0, v_j)$ *pass only through* N_1 *or only through* N_2, *then* $\partial_1(H) > \partial_1(G)$.

In the nest two theorems, Yu, Wu and Shu [144] considered the rotation of a set of edges incident to the same vertex to two different vertices: the edges satisfying a given condition to one vertex and the other edges to another vertex.

Theorem 4.31 ([144]) *Let* G *be a graph such that* $G = G_p \cup G_0 \cup G'$ *with* $G_p \cap G_0 = G_p \cap G' = G_0 \cap G' = \{v_0\}$ *and* G_p *consisting of pendent edges* $v_0v_1, v_0v_2, \ldots, v_0v_k$ $(k \ge 3)$. *Let* $S' = V(G')$ *and suppose that* $N_{G'}(v_0) =$

$N_1 \cup N_2$ satisfying that $N1 \neq \emptyset$, $N_2 \neq \emptyset$, $N_1 \cap N_2 = \emptyset$. Let

$$H = G - \sum_{v_i \in N_1} v_i v_0 - \sum_{v_i \in N_2} v_i v_0 + \sum_{v_i \in N_1} v_i v_{k-1} + \sum_{v_i \in N_2} v_i v_k.$$

If there exists vertex $v_j \in S' \setminus \{v_0\}$ such that there exist two different paths P_1 and P_2 from v_0 to v_j with the same length $d_G(v_0, v_j)$, where P_1 passes through N_1 and P_2 passes through N_2, then $\partial_1(H) > \partial_1(G)$.

Theorem 4.32 ([144]) *Let G be a graph such that $G = G_p \cup G_0 \cup G'$ with $G_p \cap G_0 = G_p \cap G' = G_0 \cap G' = \{v_0\}$ and G_p consisting of pendent edges $v_0v_1, v_0v_2, \ldots, v_0v_k$ $(k \geq 4)$. Let $S' = V(G')$ and suppose that $N_{G'}(v_0) = N_1 \cup N_2$ satisfying that $N1 \neq \emptyset$, $N_2 \neq \emptyset$, $N_1 \cap N_2 = \emptyset$. Let*

$$H = G - \sum_{v_i \in N_1} v_i v_0 - \sum_{v_i \in N_2} v_i v_0 + \sum_{v_i \in N_1} v_i v_{k-1} + \sum_{v_i \in N_2} v_i v_k.$$

For any vertex $v_j \in S' \setminus \{v_0\}$, if all paths from v_0 to v_j with a length of $d_G(v_0, v_j)$ pass only through N_1 or only through N_2, then $\partial_1(H) > \partial_1(G)$.

Now, we consider the rotation of two sets of edges incident to two different vertices. First, we consider the transformation on a tree.

Let T be an arbitrary tree and let v be a vertex with degree $p + q + 1$. Suppose that w is a parent of v and that there are p paths P_3 (two additional vertices) and q paths P_2 (pendent edges) attached at v. We form two trees T' (see Figure 37) and T'' (see Figure 38) in the following way: T' has p pendent paths P_3 and $q + 1$ pendent paths P_2 attached at w, while T'' has $p + 1$ pendent paths P_3 and $q - 1$ pendent paths P_2 attached at w. Let G be the maximal subtree of T rooted at w, that does not contain the vertex v. Thus we have the following results.

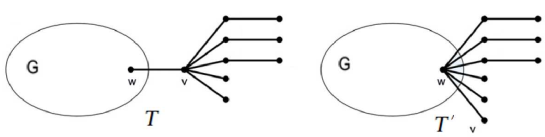

Figure 37: The transformation of T to T' in Theorem 4.33.

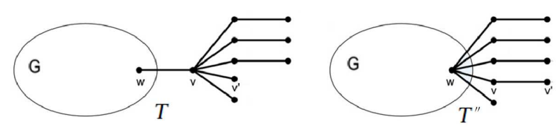

Figure 38: The transformation of T to T'' in Theorem 4.33.

Theorem 4.33 ([77]) *Let T be a tree and T' and T'' the trees obtained from T as described above and illustrated in Figure 37 and Figure 38, respectively. Let G be the maximal subtree of T rooted at w, that does not contain vertex v. Then*

- *if G is a nontrivial graph, then $\partial_1(T) > \partial_1(T')$;*
- *if G has a pendent path P_3 attached at some vertex u of G, or at least three pendent vertices, then $\partial_1(T) > \partial_1(T')$.*

A weaker version of the above theorem, where only pendent edges are considered, is proved by Ilić [76] (see also [130, 131]).

Theorem 4.34 ([76, 131]) *Let T be a tree on n vertices and consider the tree T' obtained from T as illustrated in Figure 39. Then $\partial_1(T') \leq \partial_1(T)$ with equality if and only if T (and T') is the star S_n.*

A generalization, in someway, of the above result is proved by Du, Ilić and Feng [54].

Theorem 4.35 ([54]) *Let T be a tree on n vertices and consider the tree T' obtained from T as illustrated in Figure 40, where P and Q are subtrees of T (and T'). If $d_T(u), d_T(v) \geq 2$, then $\partial_1(T) > \partial_1(T')$.*

The behavior of the distance spectral radius under the replacement of non–pendent edge by a pendent one was studied by Wang and Zhou [138]. Their result is next stated.

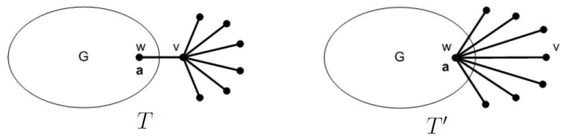

Figure 39: The transformation of T into T' in Theorem 4.34.

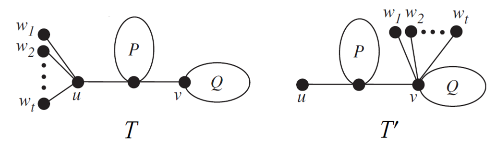

Figure 40: The transformation of T into T' in Theorem 4.35.

Theorem 4.36 ([138]) *Let G be a graph and uv be a non–pendent cut edge of G. Let G' be the graph obtained from G by contracting uv to a vertex u and attaching a pendent vertex v to u (see Figure 41). Then $\partial_1(G') < \partial_1(G)$.*

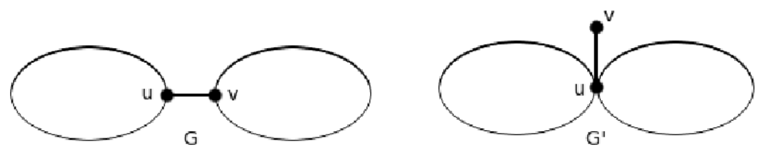

Figure 41: The transformation of G into G' in Theorem 4.36.

A *closed necklace* is a unicyclic graph, in which every vertex not on the cycle, is a pendent vertex. If G is a closed necklace with cycle $v_1v_2\cdots v_kv_1$ and m_i ($m_i \geq 0$) pendent vertices at v_i, then we denote G by $N(m_1, m_2, \ldots, m_k)$. A *chain* in a graph G is a cycle C in G, such that $G - E(C)$ has exactly $|V(C)|$ components. A *generalized closed necklace* is a graph with a chain. The length of the chain is the length of the cycle C.

Theorem 4.37 ([21]) *Let G be a generalized closed necklace with a chain of even length. If G' is the graph obtained from G by identifying two adjacent vertices on that chain, one of which has degree at least three, and creating a new pendent vertex at the identified vertex (see Figure 42), then $\partial_1(G) > \partial_1(G')$.*

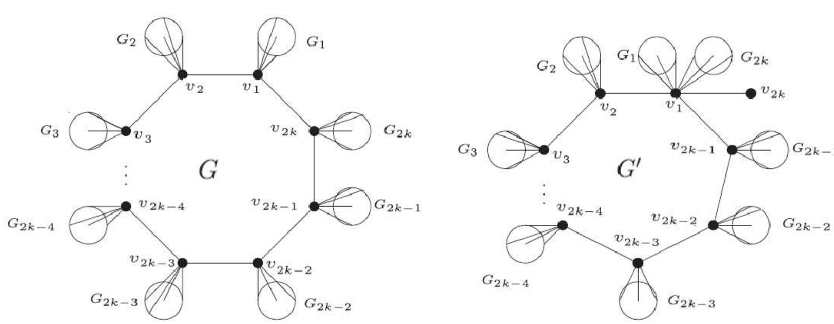

Figure 42: The graphs G and G' of Theorem 4.37.

The above theorem was generalized by the same authors to next one.

Theorem 4.38 ([21]) *Let G be a generalized closed necklace with a chain of odd length l with $l \geq 5$. If G' is the graph obtained from G by identifying three consecutive vertices on that chain, one of which has degree at least three, and creating two new pendent vertices at the identified vertex (see Figure 43), then $\partial_1(G) > \partial_1(G')$.*

In the next theorem, the rotation in question is done on three sets of edges incident to three vertices and all these edges are transformed into edges incident to the same vertex.

Theorem 4.39 ([21]) *If G and G' are the graphs as shown in Figure 44, where G_0 is non trivial. If at least one of the remaining G_i's is non trivial, then $\partial_1(G) > \partial_1(G')$.*

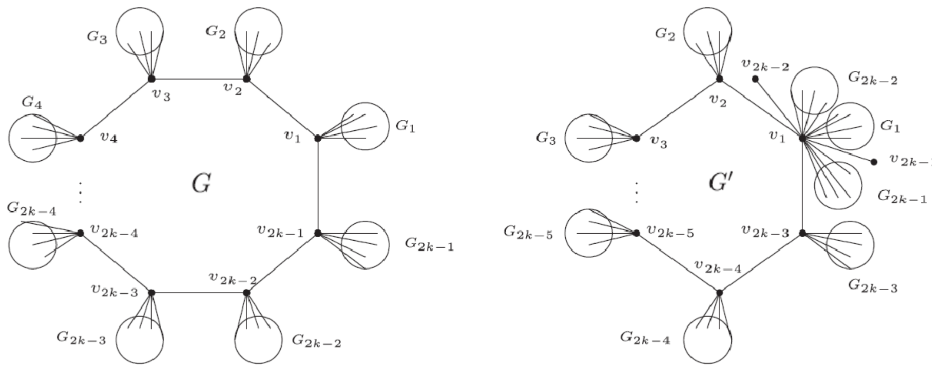

Figure 43: The graphs G and G' of Theorem 4.38.

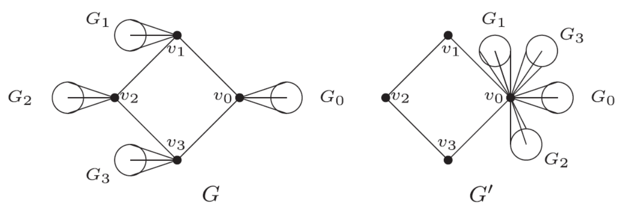

Figure 44: The graphs G and G' of Theorem 4.39.

We finish this section with a result where the considered rotation transforms several sets of pendent edges incident to different vertices to a set of pendent edges incident to a same vertex.

Theorem 4.40 ([144]) *Let G_1 be a complete graph with $V(G_1) = \{v_0, v_{k+1}, v_{k+2}, \dots, v_{n-1}\}$ $(n-k \geq 3)$. Let G be the graph consisting of G_1 and the pendent edges $v_0v_1, v_0v_2, \dots, v_0v_k$. Let H be the graph on n vertices consisting of G_1 and pendant stars S_{t_i} attached at each vertex v_i (v_i is the center of S_{t_i}) of the complete graph G_1 where stars can be trivial (with only one vertex). Then we have*

- *if $k = 0, 1$, then $\partial_1(H) = \partial_1(G)$;*
- *if $k \geq 2$ and $2 \leq t_0 \leq k$, then $\partial_1(H) > \partial_1(G)$.*

5 The largest distance eigenvalue

In the present section, we give a survey of the results related to lower or upper bounding the distance spectral radius of a graph. The bounds are expressed using several graph invariants. In most cases, the order n of the graph is involved. The problem of bounding the distance largest eigenvalue is, in some way, a recent research subject. Actually, first bounds on ∂_1 go back to the paper [116] by Ruzieh in 1990. Since then, many researchers were interested in bounding the largest distance eigenvalue of a graph. We begin with the bound proved by Ruzieh [116].

Theorem 5.1 ([116]) *If G is a graph of order n, then $n - 1 \leq \partial_1(G) \leq \partial_1(P_n)$. Moreover, the lower bound is reached if and only if G is the complete graph K_n, and the upper is reached if and only if G is the path P_n.*

In the same paper, Ruzieh computed the spectrum as well as the eigenspaces of the distance matrix of the path P_n.

Zhou and Ilić [151] proved some bounds on the distance spectral radius of a graph. First, they established a lower bound in terms of the order n, the maximum degree Δ_1 and second maximum degree Δ_2.

Theorem 5.2 ([151]) *Let G be a graph on n vertices with maximum degree Δ_1 and second maximum degree Δ_2. Then*

$$\partial_1 \geq \sqrt{(2n-2-\Delta_1)(2n-2-\Delta_2)}$$

with equality if and only if G is a regular graph with diameter less than or equal to 2.

Then, they proved an upper bound in terms of the order n, diameter D, the minimum degree δ_1 and second minimum degree δ_2.

Theorem 5.3 ([151]) *Let G be a graph on n vertices with diameter D, minimum degree δ_1 and second minimum degree δ_2. Then*

$$\partial_1 \leq \sqrt{\left(Dn - \frac{D(D-1)}{2} - 1 - \delta_1(D-1)\right)\left(Dn - \frac{D(D-1)}{2} - 1 - \delta_2(D-1)\right)}$$

with equality if and only if G is a regular graph with diameter less than or equal to 2.

Let $S = S(G)$ denote the sum of the squares of the distances between all unordered pairs of vertices in the graph, *i.e.*,

$$S = S(G) = \sum_{1 \leq i < j \leq n} d_{ij}^2.$$

Zhou and Trinajstić [153] proved a lower bound on the distance spectral radius of a graph using only the sum of the squares of the distances $S(G)$. They also proved an upper bound using the order n in addition to the sum of the squares of the distances $S(G)$. Both bounds are over the set of graphs with exactly one positive distance eigenvalue.

Theorem 5.4 ([153]) *Let G be a graph on $n \geq 2$ vertices with sum of the squares of the distances between all unordered pairs of vertices $S(G)$. If G has exactly one positive distance eigenvalue, then*

$$\partial_1(G) \geq \sqrt{S(G)}$$

with equality if and only if G is K_2, and

$$\partial_1(G) \leq \sqrt{\frac{2(n-1)S(G)}{n}}$$

with equality if and only if G is the complete graph K_n.

Note that the bounds in the above theorem, as well as the third bound in the next theorem, were first proved by Zhou [150] in the case of trees.

Zhou and Trinajstić [153] proved a series of bounds on the distance spectral radius ∂_1 of a graph in terms number of vertices n, number of edges m, Wiener index W and transmissions Tr_i, for $i = 1, \ldots, n$. These bounds are gathered in the next theorem.

Theorem 5.5 ([153]) *Let G be a graph on $n \geq 2$ vertices and m edges with Wiener index W and transmission sequence $\{Tr_1, Tr_2, \ldots, Tr_n\}$. Then*

$$\partial_1(G) \leq \max_{1 \leq i \leq n} \sum_{j=1}^{n} \mathcal{D}_{ij} \sqrt{\frac{Tr_j}{Tr_i}}$$

with equality if and only if G is a transmission regular graph;

$$\partial_1(G) \geq \sqrt{\frac{1}{n}\sum_{i=1}^{n} Tr_i^2}$$

with equality if and only if G is a transmission regular graph;

$$\partial_1(G) \geq \frac{2}{n}W(G)$$

with equality if and only if G is a transmission regular graph;

$$\partial_1(G) \geq 2(n-1) - \frac{2m}{n},$$

where m denotes the number of edges in G, with equality if and only if G is a regular graph with diameter $D \leq 2$.

Note that the second and third inequalities in the above theorem were also proved by Indulal [82].

In another paper, Zhou and Trinajstić [154] gave further bounds on the largest distance eigenvalue of a graph. The following theorem gives an upper bound on the distance spectral radius of a graph that is not transmission regular.

Theorem 5.6 ([154]) *Let G be a graph on $n \geq 2$ vertices with distance spectral radius ∂_1. Suppose the transmission sequence $\{Tr_1, Tr_2, \ldots, Tr_n\}$ is labeled such that $Tr_1 \geq Tr_2 \geq \cdots \geq Tr_n$ and $Tr_1 > Tr_{n-k+1}$ with $1 \leq k \leq n-1$. Then*

$$\partial_1 \leq \frac{Tr_1 - 1}{2} + \sqrt{\frac{(Tr_1+1)^2}{4} - k(Tr_1 - Tr_{n-k+1})}$$

with equality if and only if $k \leq n-2$, G is a graph with k vertices of degree $n-1$ and the remaining $n-k$ vertices have degree less than $n-1$.

The next theorem gives a lower bound on the distance spectral radius of a graph that is not transmission regular.

Theorem 5.7 ([154]) *Let G be a graph on $n \geq 2$ vertices with distance spectral radius ∂_1. Suppose the transmission sequence $\{Tr_1, Tr_2, \ldots, Tr_n\}$ is labeled such that $Tr_1 \geq Tr_2 \geq \cdots \geq Tr_n$ and $Tr_l > Tr_n$ with $1 \leq l \leq n-1$. Then*

$$\partial_1 > \frac{Tr_n - 1}{2} + \sqrt{\frac{(Tr_n+1)^2}{4} - l(Tr_l - Tr_n)}.$$

Combining the Wiener index W and the transmissions $\{Tr_1, Tr_2, \ldots, Tr_n\}$, Indulal [82] proved the following bound.

Theorem 5.8 ([82]) *Let G be a graph on n vertices with Wiener index W and transmission sequence $\{Tr_1, Tr_2, \ldots, Tr_n\}$. Then*

$$\partial_1(G) \geq \max_i \frac{1}{n-1}\left((W - Tr_i) + \sqrt{(W-Tr_i)^2 + (n-1)Tr_i^2}\right).$$

Indulal [82] proved a lower bound on ∂_1 using, besides the squares of the transmissions, the *second distance degree sequence*. For a vertex $v_i \in V$, the *second distance degree* is defined by

$$Tr_i^{(2)} = \sum_{j=1}^{n} d_{ij} Tr_j,$$

where d_{ij} denote the distance between v_i and v_j in G.

A graph G is said to be *pseudo k–distance regular* if $Tr_i^{(2)} = kTr_i$ for $i = 1, 2, \ldots, n$.

Theorem 5.9 ([82]) *Let G be a graph on n vertices with transmission and second distance degree sequences $\{Tr_1, Tr_2, \ldots, Tr_n\}$ and $\{Tr_1^{(2)}, Tr_2^{(2)}, \ldots, Tr_n^{(2)}\}$, respectively. Then*

$$\partial_1(G) \geq \sqrt{\frac{\sum_{i=1}^{n}\left(Tr_i^{(2)}\right)^2}{\sum_{i=1}^{n} Tr_i^2}}$$

with equality if and only if G is pseudo distance regular.

Güngör and Bozkurt [67] obtained the above theorem as a corollary of a more general result. First, they generalized the notion of transmission and second distance degree as follows. For each $i \in \{1, 2, \ldots, n\}$ and fixed real number t, define the sequence $\{M_i^{(1)}, M_i^{(2)}, \ldots, M_i^{(k)}, \ldots\}$ by

$$M_i^{(1)} = (Tr_i)^t; \qquad M_i^{(k)} = \sum_{j=1}^{n} \mathcal{D}_{i,j} M_j^{(k-1)} \quad \text{for } k \geq 2.$$

For the particular case $t = 1$, we have $M_i^{(1)} = Tr_i$ and $M_i^{(2)} = Tr_i^{(2)}$.

Theorem 5.10 ([67]) *Let G be a graph on n vertices, t be a real number and k be an integer. Then*

$$\partial_1(G) \geq \sqrt{\frac{\sum_{i=1}^{n} \left(M_i^{(k+1)}\right)^2}{\sum_{i=1}^{n} \left(M_i^{(k)}\right)^2}}.$$

Equality holds for particular values of t and k if and only if $\frac{M_1^{(k+1)}}{M_1^{(k)}} = \frac{M_2^{(k+1)}}{M_2^{(k)}} = \cdots = \frac{M_n^{(k+1)}}{M_n^{(k)}}$.

He, Liu and Zhao [71] also used the transmission and second distance degree sequences for lower and upper bounding the distance spectral radius. First, they [71] used the minimum (resp. maximum) of the ratios $Tr_i/Tr_i^{(2)}$, for $i = 1, \ldots, n$, for a lower (resp. an upper) bound.

Theorem 5.11 ([71]) *Let G be a graph on $n \geq 2$ vertices with transmission and second distance degree sequences $\{Tr_1, Tr_2, \ldots, Tr_n\}$ and $\{Tr_1^{(2)}, Tr_2^{(2)}, \ldots, Tr_n^{(2)}\}$ respectively. Then*

$$\min_{1 \leq i \leq n} \frac{Tr_i}{Tr_i^{(2)}} \leq \partial_1(G) \leq \max_{1 \leq i \leq n} \frac{Tr_i}{Tr_i^{(2)}}.$$

Moreover, any equality holds if and only if G is pseudo distance regular.

Second, they [71] used the minimum (resp. maximum) of the square roots $\sqrt{Tr_i^{(2)}}$, for $i = 1, \ldots, n$, for a lower (resp. an upper) bound.

Theorem 5.12 ([71]) *Let G be a graph on $n \geq 2$ vertices with distance spectral radius ∂_1 and second distance degree sequences $\{Tr_1^{(2)}, Tr_2^{(2)}, \ldots, Tr_n^{(2)}\}$. Then*

$$\min_{1 \leq i \leq n} \sqrt{Tr_i^{(2)}} \leq \partial_1 \leq \max_{1 \leq i \leq n} \sqrt{Tr_i^{(2)}}.$$

Moreover, any equality holds if and only if G has same value of $Tr_i^{(2)}$ for all i.

Finally, they [71] used the maximum of the square roots of the products of the transmissions and the second distance degrees $\sqrt{Tr_i \cdot Tr_i^{(2)}}$, for $i = 1, \ldots, n$, for an upper bound.

Theorem 5.13 ([71]) *Let G be a graph on $n \geq 2$ vertices with transmission and second distance degree sequences $\{Tr_1, Tr_2, \ldots, Tr_n\}$ and $\{Tr_1^{(2)}, Tr_2^{(2)}, \ldots, Tr_n^{(2)}\}$, respectively. Then*

$$\partial_1(G) \leq \max_{1 \leq i,j \leq n} \sqrt{Tr_i \cdot Tr_i^{(2)}}.$$

Moreover, any equality holds if and only if G is pseudo distance regular.

The *average distance degree* of a vertex v_i is defined as $\overline{Tr}_i = Tr_i^{(2)}/Tr_i$. Thus, a graph is pseudo k–distance regular if $\overline{Tr}_i = k$ for $i = 1, 2, \ldots, n$.

Lin and Shu [95] proved lower and upper bounds on the distance spectral radius in terms of average distance degrees.

Theorem 5.14 ([95]) *Let G be a graph on n vertices with distance spectral radius ∂_1 and average distance degree sequence $\{\overline{Tr}_1, \overline{Tr}_2, \ldots, \overline{Tr}_n\}$. Then*

$$\min_{1\leq i,j\leq n} \sqrt{\overline{Tr}_i \cdot \overline{Tr}_j} \leq \partial_1(G) \leq \max_{1\leq i,j\leq n} \sqrt{\overline{Tr}_i \cdot \overline{Tr}_j}.$$

Equalities hold if and only if G is pseudo distance regular.

Zhang [147] characterized the graphs minimizing the distance spectral radius among the class of graphs with given diameter. First, consider the following two graphs (see Figure 45). For two fixed integers n and k, whit $2k \leq n$, let H_1 be the graph obtained from two paths, each on k vertices and two cliques on $\lfloor n/2 \rfloor - k$ and $\lceil n/2 \rceil - k$ vertices respectively, by adding all possible vertices between

- an endpoint of one path and all the vertices of one clique,
- an endpoint of the other path and all the vertices of the other clique,
- each vertex of one clique and all the vertices of the other clique.

In a similar way, let H_2 be the graph obtained from two paths, each on k vertices and a clique on $n - 2k$ vertices, by adding all possible vertices between

- an endpoint of one path and all the vertices of the clique,
- an endpoint of the other path and all the vertices of the clique.

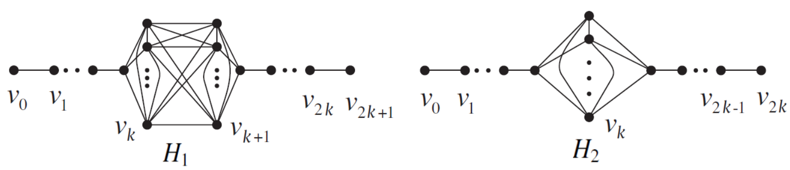

Figure 45: The graphs H_1 and H_2 in Theorem 5.15.

Theorem 5.15 ([147]) *Let G be a graph on n vertices with diameter D, and let $k = \lfloor D/2 \rfloor$. Then*

- *if $D = 2k + 1$, $\partial_1(G) \geq \partial_1(H_1)$ with equality if and only if $G \cong H_1$;*
- *if $D = 2k$, $\partial_1(G) \geq \partial_1(H_2)$ with equality if and only if $G \cong H_2$.*

A *matching* in a graph is a set of disjoint edges. The maximum possible cardinality of a matching in a graph G is called *the matching number* of G and denoted by $\mu = \mu(G)$. A matching is perfect if it contains exactly $n/2$ edges.

For the general case, Liu [98] proved that complete split graphs minimize ∂_1 among all graphs with a given matching number μ.

Theorem 5.16 ([98]) *Let G be a graphs on n vertices with matching number μ. Then*

- *if $\mu = \lfloor n/2 \rfloor$, then $\partial_1(G) \geq n - 1$ with equality if and only if $G \cong K_n$;*
- *if $2 \leq \mu \leq \lfloor n/2 \rfloor - 1$, then $\partial_1(G) \geq \partial_1(CS_{n,\mu})$, with equality if and only if $G \cong CS_{n,\mu}$.*

The complete split graphs minimize ∂_1 among all graphs with a given independence number α as shown by Ilić [76] in the next theorem.

Theorem 5.17 ([76]) *Among all graphs on n vertices with given independence number α, the complete split graph $CS_{n,n-\alpha}$ has the minimum value of distance spectral radius.*

Recall that the *chromatic number* $\chi = \chi(G)$ of a graph G is the smallest number of colors to be assigned to G's vertices such that no pair of adjacent vertices have the same color. A subset of vertices assigned to the same color is called a *color class*, every such class forms an independent set. A graph in which the vertex set can be partitioned into two independent sets is *bipartite*; three sets *tripartite*; k sets *k-partite* or *multipartite* with k independent sets. A k-partite graph is said to be complete if any two vertices are adjacent if and only if they belong to different partition classes. A k-partite graph is said to be *balanced*, and denoted by $T_k(n)$, if for any two partition classes V' and V'', $||V'| - |V''|| \leq 1$. It is also called *Turán's graph*. Liu [98] studied the problem of characterizing the graphs with minimum distance spectral radius over the class of graphs with given number n of vertices and chromatic number χ, and showed the following.

Theorem 5.18 ([98]) *Let G be a graph on n vertices with chromatic number χ, where $2 \leq \chi \leq n-1$. Then $\partial_1(G) \geq \partial_1(T_k(n))$ with equality if and only if $G \cong T_k(n)$.*

The *clique number* $\omega = \omega(G)$ of a graph G is the maximum cardinality of a clique in G. Recall that a *kite* $Ki_{n,\omega}$ is the graph obtained from a clique K_ω and a path $P_{n-\omega}$ by adding an edge between a vertex from the clique and an endpoint of the path. The problem of finding extremal values for the distance spectral radius of a graph was studied by Zhai, Yu and Shu [146].

Theorem 5.19 ([146]) *Let G be a graph on n vertices with clique number ω. Then*

$$\partial_1(T_\omega(n)) \leq \partial_1(G) \leq \partial_1(Ki_{n,\omega})$$

with equality for the lower (resp. upper) bound if and only if $G \cong T_\omega(n)$ (resp. $Ki_{n,\omega}$).

Bose, Nath and Paul [22], and Yu, Jia, Zhang and Shu [143] studied the problem of characterizing graphs minimizing the distance spectral radius on the class $\mathcal{G}_n^r$ of graphs on n vertices with r pendent vertices. First recall the following definitions. A *pineapple* with parameters n, q ($q \leq n$), denoted by $PA_{n,q}$, is a graph on n vertices consisting of a clique on q vertices and an independent set on the remaining $n-q$ vertices, in which each vertex of the independent set is adjacent to a unique and the same vertex of the clique.

Theorem 5.20 ([22, 143]) *For $n \geq 4$ and $0 \leq r \leq n-1$, there is a unique graph in $\mathcal{G}_n^r$ with minimal distance spectral radius, namely the pineapple $PA_{n,n-r}$ for $r \neq n-2$ and the double star $S_{n-2,2}$ for $r = n-2$.*

The authors of [22], as well as those of [143], were also interested in characterizing the graphs maximizing the distance spectral radius on the class $\mathcal{G}_n^r$. Their results are gathered in the next theorem.

Theorem 5.21 ([22, 143])

- *The kite $Ki_{n,3}$ is the unique graph with maximal distance spectral radius in $\mathcal{G}_n^1$, for $n \geq 4$.*
- *The path P_n is the unique graph with maximal distance spectral radius in $\mathcal{G}_n^2$, for $n \geq 3$.*
- *The comet $CO_{n,3}$ has the largest distance spectral radius in $\mathcal{G}_n^3$, for $n \geq 4$.*
- *The double comet $DC_{n,\lceil (n-1)/2\rceil,\lfloor (n-1)/2\rfloor}$ has the largest distance spectral radius in $\mathcal{G}_n^{n-3}$, for $n \geq 6$.*
- *The double star $S_{\lceil n/2\rceil,\lfloor n/2\rfloor}$ uniquely maximizes the distance spectral radius in $\mathcal{G}_n^{n-2}$, for $n \geq 4$.*

The case where r is assumed to be in an interval was solved in [143].

Theorem 5.22 ([143]) *If a graph G maximizes ∂_1 over $\mathcal{G}_n^r$ with $2 \leq r \leq n-2$, then G is a double comet $DC_{n,s+1,p+1}$.*

The above theorem was first stated for the class of trees (see Theorem 5.45 below). Finally, Yu et al. [143] made the following conjecture.

Conjecture 5.23 ([143]) *The maximum value of ∂_1 over $\mathcal{G}_n^r$, $2 \leq r \leq n-2$, is reached for the double comet $DC_{n,\lfloor r/2\rfloor,\lceil r/2\rceil}$.*

The above conjecture follows from a similar result proved by Nath and Paul [102] (see Theorem 5.51).

For the next result, we need the following definition. Let n, p, q be integers such that $n \geq p+q \geq 6$. The *double lollipop* $DL_{n,p,q}$ is the graph obtained form two cycles C_p and C_q and a path $P_{n-p-q+2}$ by the coalescence of one vertex from the cycle C_p and one endpoint of the path, and the coalescence one vertex from the cycle C_q with the other end point of the path. In the particular case where $p = q = 3$, we speak about a *double long lollipop* $DL_{n,3,3}$ [4] (see Figure 46).

After proving a series of lemmas, Bose, Nath and Paul [20] determined the family of graphs that maximize the distance spectral radius among the graphs without pending vertices, *i.e.*, over the class $\mathcal{G}_n^0$.

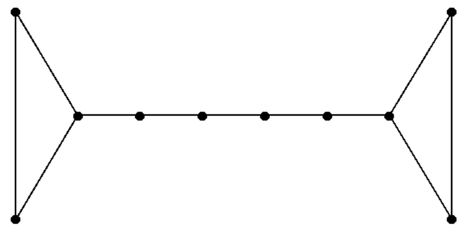

Figure 46: The double long lollipop $DL_{10,3,3}$.

Theorem 5.24 ([20]) *If $n \geq 6$, then $DL_{n,3,3}$ is the unique graph with maximal distance spectral radius in $\mathcal{G}_n^0$.*

Recall that the *vertex connectivity* of a graph G, denoted by $\nu = \nu(G)$, is the minimum number of vertices whose deletion disconnects the graph. For given integers n and ν, with $1 \leq \nu \leq n-1$, define K_{n-1}^{ν} to be the graph obtained from the complete graph K_{n-1} and an isolated vertex by adding ν edges. The lower bound on ∂_1 among all graphs with fixed vertex connectivity was proved in [98].

Theorem 5.25 ([98]) *Let G be a graph on n vertices with vertex connectivity ν. Then $\partial_1(G) \geq \partial_1(K_{n-1}^{\nu})$ with equality if and only if G is the graph K_{n-1}^{ν}.*

For $\nu = 1$, as a result of Theorem 5.1, P_n is the only graph that maximizes ∂_1. For $\nu = 2$, Lin et al. [96] proved that the maximum of ∂_1 is reached only for the cycle C_n.

Recall that the *edge connectivity* of a graph G, denoted by $\kappa = \kappa(G)$, is the minimum number of vertices whose deletion disconnects the graph. Li, Fan and Wang [94] characterized the graphs that minimize the distance spectral radius with given order n and edge connectivity κ.

Theorem 5.26 ([94]) *For given integer κ and n such that $1 \leq \kappa \leq n-1$, the graph K_{n-1}^{κ} is the unique graph with minimum distance spectral radius among the graphs on n vertices with edge connectivity κ.*

Zhang and Godsil [149] studied the problem of characterizing the graphs with k cut vertices (resp. edges) with minimum distance index.

Let $G_{n,k}$ be the graph obtained by adding paths $P_{l_1+1}, \ldots, P_{l_{n-k}+1}$ of almost equal lengths, *i.e.* such that $|l_i - l_j| \leq 1$ for all $1 \leq i, j \leq n-k$, to the vertices of the complete graph K_{n-k}.

Zhang and Godsil [149] used Theorem 4.17 to prove the next result.

Theorem 5.27 ([149]) *Of all the graphs with n vertices and k cut vertices, the minimal distance spectral radius is obtained uniquely at $G_{n,k}$.*

Again in [149], the authors used Theorem 4.24 to characterize the graphs minimizing the distance index when the numbers of vertices and cut edges are fixed.

Theorem 5.28 ([149]) *Of all the graphs with $n \geq 4$ vertices and k cut edges, the minimal distance spectral radius is obtained uniquely at the pineapple $PA_{n,n-k}$.*

Now, we consider the problem of lower and upper bounding the distance spectral radius over the class of bipartite graphs.

Zhou and Ilić [151] characterized extremal graphs for the lower bound on ∂_1 over all bipartite graphs with given number of vertices.

Theorem 5.29 ([151]) *Among bipartite graphs with n vertices, $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ has minimum distance spectral radius.*

In addition to the order n, Das [46] used the cardinalities of the partition sets of a bipartite graph to obtain a lower bound on its distance spectral radius.

Theorem 5.30 ([46]) *Let G be a bipartite graph with bipartition $V(G) = A \cup B$ with $|A| = p$, $|B| = q$ and $p+q = n$. Then*

$$\partial_1(G) \geq n - 2 + \sqrt{n^2 - 3pq}$$

with equality if and only if G is a complete bipartite graph $K_{p,q}$.

Zhou and Ilić [151] added the maximum degrees within the partition sets to their cardinalities and the order to improve the lower bound on ∂_1 provided in the above theorem.

Theorem 5.31 ([151]) *Let G be a bipartite graph with bipartition $V(G) = A \cup B$ with $|A| = p$, $|B| = q$ and $p+q = n$. Let Δ_A and Δ_B be maximum degrees among vertices from A and B, respectively. Then*

$$\partial_1(G) \geq n - 2 + \sqrt{n^2 - 4pq + (3q - 2\Delta_A)(3p - 2\Delta_B)}$$

with equality if and only if G is a complete bipartite graph $K_{p,q}$ or G is a semi–regular graph with every vertex eccentricity equal to 3.

To the parameters used in Theorem 5.30, Das [46] added the diameter D to prove an upper bound on the distance spectral radius of a bipartite graph.

Theorem 5.32 ([46]) *Let G be a bipartite graph on n vertices with diameter D, minimum degree δ and bipartition $V(G) = A \cup B$ such that $|A| = p$, $|B| = q$. Then*

$$\partial_1(G) \leq \frac{1}{2}\left(D(n-2) + \sqrt{D^2n^2 - 4pq(2D-1)}\right)$$

for even D, and

$$\partial_1(G) \leq \frac{1}{2}\left((D-1)(n-2) + \sqrt{(D-1)^2n^2 - 4(D-1)^2(pq - \delta^2) + 4D^2pq - 4D(D-1)\delta n}\right)$$

for odd D. Moreover, the equality holds in the case of even D if and only if G is the complete bipartite graph $K_{p,q}$.

Again, Zhou and Ilić [151] added the minimum degrees δ_A and δ_B within the partition sets of a bipartite graph to improve the bounds given in Theorem 5.32.

Theorem 5.33 ([151]) *Let G be a bipartite graph on n vertices with diameter D and bipartition $V(G) = A \cup B$ such that $|A| = p$, $|B| = q$. Let δ_A and δ_B be minimum degrees among vertices from A and B, respectively. Then*

$$\partial_1 \leq \frac{D(n-1)}{2} - \frac{D^2}{4} + \frac{\sqrt{D^2n^2 + 4\delta_A\delta_B(D-2)^2 - 4pq(2D-1) - 4(D-1)(D-2)(p\delta_A + q\delta_B)}}{2}$$

for even D, and

$$\partial_1 \leq \frac{D(n-1)+1}{2} - \frac{D^2}{4} + \frac{\sqrt{(D-1)^2n^2 + 4\delta_A\delta_B(D-1)^2 - 4pq(2D-1) - 4D(D-1)(p\delta_A + q\delta_B)}}{2}$$

for odd D.

The problem of finding the extremal values of the distance spectral radius over the class of bipartite graphs with a fixed invariant was also considered by Nath and Paul [103]. They studied the cases fixed matching, independence, vertex covering and edge covering numbers. A *vertex* (resp. *edge*) *cover* of a graph G is a set of vertices (resp. edges) such that each edge (resp. vertex) of G is incident with at least one vertex (resp. edge) of the set. The *vertex* (resp. *edge*) *cover number* of G, denoted by $\beta = \beta(G)$ (resp $\beta' = \beta'(G)$), is the minimum cardinality over all vertex (resp. edge) covers. The results proved in [103] are next gathered.

Theorem 5.34 ([103]) *The complete bipartite graph $K_{k,n-k}$ is the unique graph that minimizes the distance spectral radius among the bipartite graphs on n vertices with given matching number, independence number, vertex covering number or edge covering number k.*

Note that for any bipartite graph G, from König's theorem [88], $\alpha(G) = \beta'(G)$ and $\mu(G) = \beta(G)$. Thus, the above theorem can be restricted to independence and matching numbers.

For $k = 1, \ldots, 4$ and any integers p and s with $s \le p$, consider the bipartite graph $B_{p,p+k,s}$ obtained from the complete bipartite graph $K_{p,p+k-1}$ and an isolated vertex v by adding s edges between v and s vertices from the partition of $K_{p,p+k-1}$ that contains p vertices. Nath and Paul [103] considered the problem of finding a lower bound on ∂_1 over the class of bipartite graphs with fixed vertex connectivity.

Theorem 5.35 ([103]) *Let G be a bipartite graph on $n = 2p + k$ vertices, where $1 \le k \le 4$, with fixed vertex connectivity $\nu = s$. Then*

$$\partial_1(G) \ge \partial_1(B_{p,p+k,s})$$

with equality if and only if $G \cong B_{p,p+k,s}$.

We consider now the problem of bounding the distance spectral radius over the class of trees.

Among the first bounds on the largest distance eigenvalue of graphs, the lower and upper bounds proved by Gutman and Medeleanu [68] over the class of trees.

Theorem 5.36 ([68]) *Let T be a tree on n vertices. Denote by S the sum of the squares of all the distances between all unordered pairs of vertices of T. Then*

$$\sqrt{\frac{1}{2}S + n(n-1)\left(\frac{n-1}{4}\right)^{\frac{2}{n}}} \le \partial_1(T) \le \sqrt{\frac{n-1}{2}S + n\left(\frac{n-1}{4}\right)^{\frac{2}{n}}}.$$

In [131], Stevanović and Ilić used an operation on trees that increases the value of the distance spectral radius (see Theorem 4.34) to give a new proof of Theorem 5.1 (first proved in [116]). They used the same technique to prove an upper bound on ∂_1 over the class of trees with given order n and maximum degree Δ. They also characterized the corresponding extremal trees.

Theorem 5.37 ([131]) *Let T be a tree on n vertices with maximum degree Δ such that $T \ncong CO_{n,\Delta}$. Then*

$$\partial_1(T) < \partial_1(CO_{n,\Delta}).$$

Ilić [76] (see also [54, 131]) ordered the double stars according to their distance spectral radius.

Theorem 5.38 ([54, 76, 130]) *Let a and b be two integer with $a \ge b \ge 1$. Then*

$$\partial_1(S_{a,b}) > \partial_1(S_{a+1,b-1}).$$

The above result was used by Du, Ilić and Feng [54] to characterize the trees with the three first minimal distance spectral radii.

Theorem 5.39 ([54]) *Let T be a tree on $n \ge 6$ vertices such that $T \notin \{S_{n-1,1}, S_{n-2,2}, S_{n-3,3}\}$. Then*

$$\partial_1(T) > \partial_1(S_{n-3,3}) > \partial_1(S_{n-2,2}) > \partial_1(S_{n-1,1}).$$

Ilić [76] and Stevanović and Ilić [131] also investigated the problem of finding lower bounds on the distance spectral radius over the class of trees. Their first lower bound was expressed in terms of the order n.

Theorem 5.40 ([76, 131]) *Let T be a tree on n vertices. Then*

$$\partial_1(T) \ge n - 2 + \sqrt{(n-2)^2 + (n-1)}$$

with equality if and only if T is the star S_n.

Stevanović and Ilić [131] also proved a lower bound on ∂_1 over the class of starlike trees. A Δ–*starlike tree* $T(n_1, n_2, \ldots, n_\Delta)$ is a tree that consists of a root vertex v, and Δ paths $P^1, P^2, \ldots, P^\Delta$ of lengths $n_1, n_2, \ldots, n_\Delta$ attached at v. Therefore, the number of vertices of $T(n_1, n_2, \ldots, n_\Delta)$ is $n = n_1+n_2+\cdots+n_\Delta+1$. The Δ–starlike tree is *balanced* if all paths have almost equal lengths, *i.e.*, $|n_i - n_j| \leq 1$ for every $1 \leq i, j \leq \Delta$ (see Figure 47 for the balanced starlike tree $T(5, 4, 4, 4)$). Note that the broom or comet $CO_{n,\Delta}$ is the Δ–starlike tree $T(1, 1, \ldots, 1, n - \Delta - 1)$, which is balanced if and only if $\Delta = n - 2$ or $\Delta = n - 1$. The case $\Delta = n - 1$ corresponds to the star S_n.

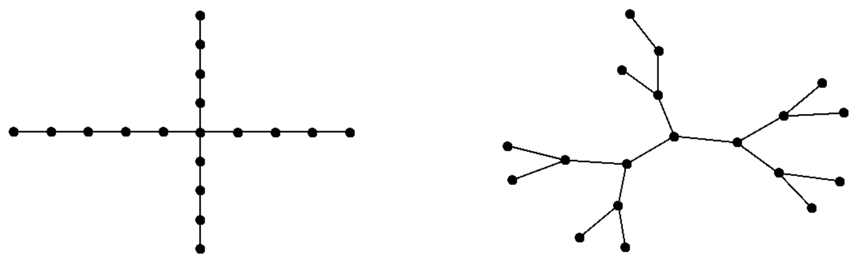

Figure 47: The balanced starlike tree $T(5, 4, 4, 4)$ on 18 vertices and the complete 3–ary tree on 19 vertices.

Theorem 5.41 ([131]) *The balanced Δ–starlike tree has the minimum distance spectral radius among Δ–starlike trees of order n.*

The *complete Δ–ary tree* is a tree on n vertices with maximum degree Δ constructed as follows. Fix a vertex to be a root. The root composes the level 0. Form level 1 by adding Δ neighbors (children) to the root. Form level 2 by adding $\Delta - 1$ children to each vertex of level 1. We continue the construction of the levels till the n vertices are attached and such that (i) all the vertices that do not belong to the two last levels have degree Δ, (ii) at most one vertex of the level before the last one has degree different from Δ and from 1, and and all the remaining vertices are pendent (see Figure 47 for the complete 3–ary tree on 19 vertices).

Finally, Stevanović and Ilić [131] conjectured that the Δ–ary trees minimizes ∂_1 over the class of trees on n vertices with maximum degree Δ.

Conjecture 5.42 ([131]) *The complete Δ–ary tree has the minimum distance spectral radius ∂_1 among all trees on n vertices with maximum degree Δ.*

Note that the authors of the above conjecture showed it to be true for trees on up to 24 vertices using computational experiments.

The problem of bounding the distance spectral radius over the set of trees with given order and diameter, was partially solved by Du, Ilić and Feng [54] and [148].

Theorem 5.43 ([54, 148]) *Among trees with n vertices and even diameter D, where $2 \leq D \leq n - 1$, $T_{n,D}$ is the unique tree with minimal distance spectral radius, where $T_{n,D}$ is the tree obtained from a path $P = v_0 v_1 \cdots v_D$ by attaching $n - D - 1$ pendent vertices to the vertex $v_{\frac{D}{2}}$.*

For the case on an odd diameter, only a conjecture is stated by the authors of [54] and [148].

Conjecture 5.44 ([54, 148]) *Among trees with n vertices and odd diameter D, where $3 \leq D \leq n - 1$, $T_{n,D}$ is the unique tree with minimal distance spectral radius, where $T_{n,D}$ is the tree obtained from a path $P = v_0 v_1 \cdots v_D$ by attaching $n - D - 1$ pendent vertices to the vertex $v_{\lfloor \frac{D}{2} \rfloor}$.*

The investigations of Yu, Jia, Zhang and Shu [143] on the problem of finding an upper bound on the distance spectral radius over all trees on n vertices with fixed number of pendent vertices led to the following result.

Theorem 5.45 ([143]) *The maximum of ∂_1 over all trees on n vertices r pendent vertices ($2 \leq r \leq n - 2$) is reached for a double comet $DC_{n,s,p}$ for some integers s and p with $r = s + p$.*

Note that the above result was also proved by Du, Ilić and Feng [54].

The problem of finding a lower bound on the spectral radius over the set of trees with fixed order n and number of pendent vertices r was solved by Du, Ilić and Feng [54], and Ning, Ouyang and Lu [105]. They independently proved the next theorem.

Theorem 5.46 ([54, 105]) *Let T be a tree on $n \geq 6$ vertices with $r \geq 3$ pendent vertices. Then $\partial_1(T) \geq \partial_1(ST(l_1, l_2, \ldots, l_r))$, where $ST(l_1, l_2, \ldots, l_r)$ is the r-starlike tree with $\lfloor (n-1)/r \rfloor \leq l_i \leq \lceil (n-1)/r \rceil$ for $i = 1, 2, \ldots, r$. Moreover, equality holds if and only if $T \cong ST(l_1, l_2, \ldots, l_r)$.*

A *spur* $Sp_{n,p}$ is the tree on n ($n \geq 2p$) vertices obtained from the star S_{n-p+1} by attaching a pendent vertex to each of $p-1$ non–central vertices of S_{n-p+1}. In fact, the spur $p_{n,p}$ is the balanced $n-p$–starlike tree with $n \geq 2p$. Note that the matching number of a spur $Sp_{n,p}$ is $\mu = p$. It is known [75] that the spur $Sp_{n,\mu}$ is the only graph maximizing the (adjacency) spectral radius among the class of trees on n vertices with matching number μ. Ilić [77] studied the problem of finding extremal values of the distance spectral radius on the class of tree with given order n and matching number μ. For the minimum, he proved the following result.

Theorem 5.47 ([77]) *Let T be a tree on $n \geq 3$ vertices with matching number μ. Then*

$$\partial_1(T) \geq \partial_1(Sp_{n,\mu})$$

with equality if and only if $T \cong Sp_{n,\mu}$.

It is well–known that for a bipartite graph on n vertices with matching number μ and independence number α, $\mu + \alpha = n$ (a consequence of König's Theorem [88]). Thus the next results follows immediately from the above theorem.

Corollary 5.48 ([77]) *Among trees on n vertices and with independence number α, $Sp_{n,n-\alpha}$ is the unique tree that has minimal distance spectral radius.*

Instead of applying the condition of a fixed maximum degree to the class of all trees, Ilić [77] considered it on restricted class of trees with a perfect matching. He proved the following theorem.

Theorem 5.49 ([77]) *Among trees on n vertices with perfect matching and maximum degree Δ, the starlike tree $T(1, n-2\Delta+2, 2, 2, \ldots, 2)$ has maximal distance spectral radius.*

After experimental results on the set of all trees on at most 24 vertices, Ilić [77] stated a conjecture about the trees that maximize ∂_1 when the order and the matching number are fixed. The conjecture was proved by Nath and Paul [102] in the next theorem.

Theorem 5.50 ([102]) *Over all trees on n vertices with matching number μ, the dumbbell DC_{n,Δ_1,Δ_2} is the unique tree that maximizes the distance spectral radius, where*

$$\Delta_1 = \left\lceil \frac{n+1}{2} \right\rceil - \mu + 1 \qquad \textit{and} \qquad \Delta_2 = \left\lfloor \frac{n+1}{2} \right\rfloor - \mu + 1.$$

Besides the above theorem, Nath and Paul [102] proved that the dumbbells also maximize the ∂_1 over trees with given order and number of pendent vertices.

Theorem 5.51 ([102]) *Over all trees of order n with p pendent vertices, the dumbbell DC_{n,Δ_1,Δ_2} is the unique tree that maximizes the distance spectral radius, where*

$$\Delta_1 = \left\lceil \frac{p}{2} \right\rceil + 1 \qquad \textit{and} \qquad \Delta_2 = \left\lfloor \frac{p}{2} \right\rfloor + 1.$$

In order to prove Theorem 5.50 and Theorem 5.51, Nath and Paul [102] first proved Theorems 3.12 and 3.13 as well as the next lemma, that gives an ordering of the dumbbells with same number of pendent vertices, according to their distance spectral radii.

Lemma 5.52 ([102]) *If $k \geq 3$, then*

- $\partial_1(DC_{n,k,k}) > \partial_1(DC_{n,k+1,k-1}) > \cdots > \partial_1(DC_{n,2k-2,2})$;
- $\partial_1(DC_{n,k+1,k}) > \partial_1(DC_{n,k+2,k-1}) > \cdots > \partial_1(DC_{n,2k-1,2})$.

Regarding the ordering of the double comets using their distance spectral radii, Wang and Zhou [138] completed, in someway, the above lemma with the following result.

Theorem 5.53 ([138]) *Let n, m_1 and m_2 be integers such that $m_1 < m_2 < n/2 - 1$. Then*

$$\partial_1\left(DC_{n,\lceil\frac{n+1}{2}\rceil-m_1,\lfloor\frac{n+1}{2}\rfloor-m_1}\right) < \partial_1\left(DC_{n,\lceil\frac{n+1}{2}\rceil-m_2,\lfloor\frac{n+1}{2}\rfloor-m_2}\right).$$

A *dominating set* of a graph G is a set S of vertices such that each vertex in $V(G) \setminus S$ is adjacent to at least one vertex in S. For a graph G, the minimum cardinality of a dominating set is called the *domination number* of G and is denoted by $\gamma(G)$. Denote by $ST_{n,m}$ the $n-m$–starlike $T(\underbrace{2,\ldots,2}_{m-1},\underbrace{1,\ldots,1}_{n-2m+1})$. It is easy to see that $\gamma(ST_{n,m}) = m$.

Wang and Zhou [138] investigated the problem of bounding the distance spectral radius of trees with given order and domination number. For the lower bound, they proved the next theorem.

Theorem 5.54 ([138]) *Let T be a tree on n vertices with domination number γ. Then $\partial_1(T) \geq \partial_1(ST_{n,\gamma})$ with equality if and only if T is the starlike $ST_{n,\gamma}$.*

The problem of upper bound is solved in the next result. First, we need some definitions. A *caterpillar* is the tree in which removal of all pendent vertices gives a path. For integers n, a and b such that $n \geq 2(a+b)$, denote by $CA_{n,a,b}$ the particular caterpillar obtained from a path $P = v_1v_2\cdots v_{n-a-b}$ by attaching a pendent edge to each of the a first vertices of P, and a pendent edge to each of the b last vertices of P.

Theorem 5.55 ([138]) *Let T be a tree on n vertices with domination number γ.*

- *If $1 \leq \gamma < \lceil n/3 \rceil$, then*
$$\partial_1(T) \leq \partial_1\left(DC_{n,\lceil\frac{n-3\gamma+2}{2}\rceil,\lfloor\frac{n-3\gamma+2}{2}\rfloor}\right)$$
with equality if and only if T is the double comet $DC_{n,\lceil\frac{n-3\gamma+2}{2}\rceil,\lfloor\frac{n-3\gamma+2}{2}\rfloor}$.
- *If $\lceil n/3 \rceil < \gamma \leq \lfloor n/2 \rfloor$, then*
$$\partial_1(T) \leq \partial_1\left(CA_{n,\lceil\frac{3\gamma-n}{2}\rceil,\lfloor\frac{3\gamma-n}{2}\rfloor}\right)$$
with equality if and only if T is the caterpillar $CA_{n,\lceil\frac{3\gamma-n}{2}\rceil,\lfloor\frac{3\gamma-n}{2}\rfloor}$.

The validity of the upper bound in the above theorem was extended [138] to the class of all connected graphs on n vertices with domination number γ such that $1 \leq \gamma < \lceil n/3 \rceil$.

To prove the above theorem, Wang and Zhou [138] used Theorem 3.14 as well as the next two lemmas.

Lemma 5.56 ([138]) *Let n, a and b be integers with $n \geq 2(a+b)$. Then*

$$\partial_1(CA_{n,a+1,b-1}) > \partial_1(CA_{n,a,b}).$$

Lemma 5.57 ([138]) *Let T be a caterpillar of order n with p pendent vertices such that $2 \leq p \leq \lfloor n/2 \rfloor$ and each vertex of T has at most one pendent neighbor. Then*

$$\partial_1(T) \leq \partial_1\left(CA_{n,\lceil\frac{p}{2}\rceil,\lfloor\frac{p}{2}\rfloor}\right)$$

with equality if and only if T is the caterpillar $CA_{n,\lceil\frac{p}{2}\rceil,\lfloor\frac{p}{2}\rfloor}$. Also, for $p_1 > p_2$,

$$\partial_1\left(CA_{n,\lceil\frac{p_1}{2}\rceil,\lfloor\frac{p_1}{2}\rfloor}\right) < \partial_1\left(CA_{n,\lceil\frac{p_2}{2}\rceil,\lfloor\frac{p_2}{2}\rfloor}\right).$$

Du, Ilić and Feng [54], and Wang and Zhou [138] considered also the problem of bounding the distance spectral radius of trees with fixed bipartition size (number of vertices in each partition).

Theorem 5.58 ([54, 138]) *Let T be a tree with bipartition size (p, q) such that $2 \leq p \leq q$. Then*

$$\partial_1(T) \geq \partial_1(DC_{p+q,p,q})$$

with equality if and only if T is the double comet $DC_{p+q,p,q}$. Moreover, if $p \leq q-2$, then

$$\partial_1(T) \leq \partial_1\left(DC_{p+q,\lceil\frac{q-p+3}{2}\rceil,\lfloor\frac{q-p+3}{2}\rfloor}\right)$$

with equality if and only if T is the double comet $DC_{p+q,\lceil\frac{q-p+3}{2}\rceil,\lfloor\frac{q-p+3}{2}\rfloor}$.

The validity of the upper bound in the above theorem was extended [138] to the class of all connected bipartite graphs with fixed bipartition size.

We saw above that over the class of all trees on n vertices, the distance spectral radius is maximum only for the path P_n (see Theorem 5.1) and is minimum only for the star S_n (see Theorem 5.40). The natural extention of these results, namely the characterization of the extremal trees with the second and third minimum and maximum values of the distance spectral radius, was investigated by Wang and Zhou [138]. Regarding the second minimum and maximum values, they proved the following.

Theorem 5.59 ([138]) *Let T be a tree on $n \geq 5$ vertices such that $T \ncong S_n$ and $T \ncong P_n$. Then $\partial_1(CO_{n,n-2}) \leq \partial_1(T) \leq \partial_1(CO_{n,3})$ with equality if and only if T is the comet $CO_{n,n-1}$ for the lower bound, and if and only if T is the comet $CO_{n,3}$ for the upper bound.*

Note that the upper bound in the above theorem can be seen as a corollary of Theorem 5.37.

Regarding the third minimum and maximum value of ∂_1, Wang and Zhou used Theorem 4.23 to prove the following result.

Theorem 5.60 ([138]) *Let T be a tree on $n \geq 6$ vertices such that $T \notin \{S_n, P_n, CO_{n,n-2}, CO_{n,3}\}$. Then $\partial_1(S_{n-3,3}) \leq \partial_1(T) \leq \partial_1(T_n)$, where T_n is the tree obtained from a path $P = v_1v_2v_3\ldots v_{n-1}$ by attaching a pendent vertex v_n to v_3, with equality if and only if T is the double star $S_{n-3,3}$ for the lower bound, and if and only if T is T_n for the upper bound.*

After a survey of the results related to the broblem of bounding the distance spectral radius over general graphs, bipartite graphs and trees, we turn to some particular classes of graphs.

A *lollipop* $L_{n,p}$ is the unicycle graph obtained from a a cycle C_p and and a path P_{n-p} by adding an edge between an endpoint of the path and a vertex form the cycle. $L_{n,3}$ is called the *long lollipop* and illustrated in Figure 48 in the case $n = 8$. Yu, Wu, Zhang and Shu [144] characterized the extremal graphs for ∂_1 over the *unicyclic* graphs *i.e.*, connected graphs on n vertices with n edges.

Theorem 5.61 ([144]) *Let G be a unicyclic graph on $n \geq 4$ vertices. Then we have*

- *if $n \geq 6$, $\partial_1(G) \geq \partial_1(PA_{n,3})$ with equality if and only if G is the pineapple $PA_{n,3}$;*
- *if $n = 4, 5$, $\partial_1(G) \geq \partial_1(C_n)$, with equality if and only if $G \cong C_n$;*
- *$\partial_1(G) \leq \partial_1(L_{n,3})$ with equality if and only if G is the long lollipop $L_{n,3}$.*

Paul [108] investigated the problem of upper bounding the distance spectral radius of a *bicyclic graph*, *i.e.*, a connected graph containing exactly two cycles.

Theorem 5.62 ([108]) *The bicyclic graph graph obtained by attaching a path on $n-4$ vertices at a vertex of degree 2 of a $K_4 - e$ (see Figure 49) is the unique graph with maximal distance spectral radius over the class of all bicyclic graph on $n \geq 5$ vertices.*

To prove the above theorem, Paul first proved that the bicyclic graph maximizing ∂_1 must contain $K_4 - e$ as an induced subgraph, and then used lemmas among which Theorem 4.15 and Theorem 4.17.

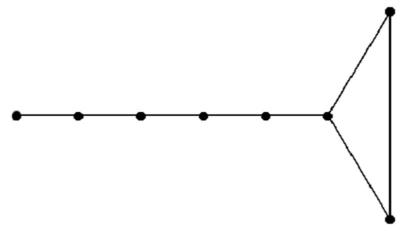

Figure 48: The long lollipop $DL_{8,3}$.

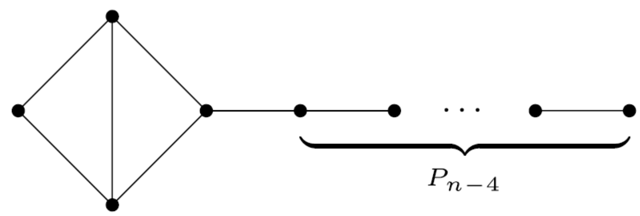

Figure 49: The bicyclic graph in Theorem 5.62

The *first Zagreb index* $M_1(G)$ is defined to be the sum of squares of the degrees of all vertices in G, *i.e.*

$$M_1(G) = \sum_{i=1}^{n} d_i^2.$$

Zhou and Trinajstić [153] proved a lower bound on $\partial_1(G)$ in terms of n, m and $M_1(G)$ for the class of triangle–free and quadrangle–free graphs, *i.e.*, graphs that do not contain C_3 or C_4.

Theorem 5.63 ([153]) *Let G be a triangle–free and quadrangle–free graph with $n \geq 2$ vertices and m edges. Then*

$$\partial_1(G) \geq 3(n-1) - \frac{M_1(G)}{n} - \frac{2m}{n}$$

with equality if and only if G is a transmission regular graph with diameter at most 3.

A *hexagonal system* is a 2–plane graph every interior face of which is bounded by a regular hexagon of unit length. A vertex of a hexagonal system belongs to, at most, three hexagons. A vertex shared by three hexagons is called an *internal vertex* of the respective hexagonal system. A hexagonal system H is said to be *catacondensed* if it does not possess internal vertices, otherwise H is said to be *pericondensed*. A *hexagonal chain* is a catacondensed hexagonal system which has no hexagon adjacent to more than two hexagons. A linear hexagonal chain denoted by L_h is a chain of h hexagons arranged in a linear manner. Zhang [147] characterized the graph with maximum distance spectral radius among the hexagonal systems with a fixed number of hexagons.

Theorem 5.64 ([147]) *Among all the catacondensed hexagonal systems on h hexagons, the linear hexagonal chain L_h has the maximum distance spectral radius.*

A *cactus* is a graph in which any two cycles have at most one common vertex. If all the cycles in a cactus have exactly one common vertex, then the graph is called a *bundle*. Let $C(n, k)$ be a bundle of k triangles and $n - 2k - 1$ pendent vertices all attached at the common vertex.

Theorem 5.65 ([21]) *If $n \geq 6$, then $C(n, k)$ minimizes the distance spectral radius among all cacti on n vertices with k cycles.*

The proof of the above theorem uses Theorems 4.25, 4.37 and 4.38. The technique of the proof led to the following corollary.

Corollary 5.66 ([21]) *If $n \geq 6$, then $\{C(n,k)|k = \lfloor \frac{n}{2} \rfloor, \lfloor \frac{n}{2} \rfloor - 1, \ldots, 2, 1, 0\}$ is the sequence of graphs with $1^{st}, 2^{nd}, \ldots, (\lfloor \frac{n}{2} \rfloor + 1)^{th}$ smallest distance spectral radius, respectively, among the class of all cacti on n vertices.*

Theorem 5.67 ([21]) *Among the cacti of order n with r pendent vertices, the graph with minimal distance spectral radius is G_0, when the parities of n and r are different; and G_1, when the parities of n and r are the same, where G_0 and G_1 are the graphs as shown in Figure 50.*

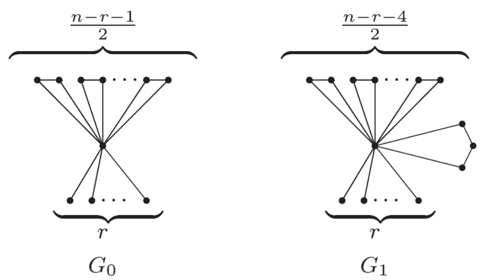

Figure 50: The graphs G and G' of Theorem 5.67.

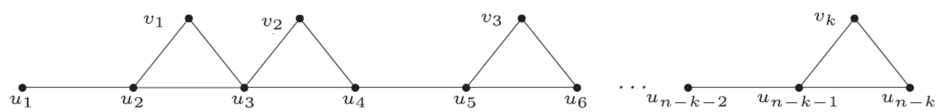

Figure 51: A saw graph.

A *saw graph* of order n and length k is a cactus obtained from a path P_{n-k} by replacing k of its blocks by k triangles, where $0 \leq k \leq \lfloor (n-1)/2 \rfloor$ (see Figure 51). A saw graph of length k and order $2k+1$ is a *proper saw graph*. An *end* in a proper saw graph is a vertex of degree 2, with a neighbor of degree 2. The saw graph obtained by joining an end of a proper saw graph of length p with an end of another proper saw graph of length q by a path of length l is denoted by $Sw(p,q;l)$. If $l = 0$, then we have the proper saw graph of length $p+q$. Note that the P_n is a saw graph of length 0.

Theorem 5.68 ([21]) *If G is a graph with maximal distance spectral radius in among the class of cacti on n with k triangles, then $G \cong Sw(p,q;l)$ for some p and q such that $p+q=k$ and where $l = n-2k-1$.*

Concerning the values of p and q (in the above theorem) for which the distance spectral radius is reached Bose et al. [21] conjectured the following.

Conjecture 5.69 ([21]) *$Sw(\lfloor k/2 \rfloor, \lceil k/2 \rceil; 2n-k-1)$ uniquely maximizes the distance spectral radius among all cacti on n vertices with k triangles.*

To end this section, we state some Nordhaus–Gaddum type inequalities for distance spectral radius. First, what a Nordhaus–Gaddum type inequality is?

In 1956, Nordhaus and Gaddum [106] gave lower and upper bounds on the sum and the product of the chromatic number of a graph and its complement, in terms of the order of the graph, namely, the following theorem.

Theorem 5.70 ([106]) *If G is a graph of order n, then*

$$2\sqrt{n} \leq \chi(G) + \chi(\overline{G}) \leq n+1 \quad \text{and} \quad n \leq \chi(G) \cdot \chi(\overline{G}) \leq \frac{(n+1)^2}{4}.$$

Furthermore, these bounds are best possible for infinitely many values of n.

Since then, relations of a similar type are called Nordhaus–Gaddum type inequalities and have been proposed for many other graph invariants, in several hundred papers. For a survey of such inequalities see [6].

Zhou and Trinajstić [153] proved Nordhaus–Gaddum type inequalities for the distance spectral radius of a graph and its complement.

Theorem 5.71 ([153]) *Let G be a graph on $n \geq 4$ vertices with a connected complement $\overline{G}$. Then*

$$3(n-1) \leq \partial_1(G) + \partial_1(\overline{G}) < \frac{n(n+3)}{2} - 3$$

with left equality if and only if G and $\overline{G}$ are both regular graphs of diameter two. Moreover, if G or $\overline{G}$ has exactly one positive distance eigenvalue, then

$$\partial_1(G) + \partial_1(\overline{G}) < \sqrt{\frac{(n+1)n(n-1)^2}{6}} + 2n - 3.$$

The lower bound in the above theorem can be obtained as a corollary of a more general lower bound involving, besides the order n, the diameter D. Actually, this bound is proved by Das [45].

Theorem 5.72 ([45]) *Let G be a graph, with a connected complement, on $n \geq 4$ vertices with diameter D. Then*

$$\partial_1(G) + \partial_1(\overline{G}) \geq 3(n-1) + \frac{D(D-1)(D-2)}{3n} \geq 3(n-1)$$

with equality if and only if G and $\overline{G}$ are both regular graphs with diameter 2.

6 The distance spectral spread

The *distance spectral spread* $s_D(G)$ of a graph G is the difference between its largest and smallest eigenvalues, *i.e.*, $s_D(G) = \partial_1(G) - \partial_n(G)$. Yu, Zhang, Lin, Wu and Shu [145] studied the problem of bounding the distance spectral spread of a graph. This problem remains to be explored.

The first result about the distance spectral spread is a lower bound in terms of the order n, maximum degree Δ, Wiener index W and average distance degree $\overline{Tr}_i$ with $1 \leq i \leq n$.

Theorem 6.1 ([145]) *Let G be a graph on n vertices with maximum degree Δ and Wiener index W. Suppose that the vertices of G are labeled such that the degree sequence satisfies $d_1 = d_2 = \cdots = d_k = \Delta > d_{k+1} \geq d_{k+2} \geq \cdots \geq d_n$, for some k. He have:*

(i) if $\Delta \leq n-2$, then

$$s_D \geq \max_{1 \leq i \leq k} \frac{\sqrt{x_i^2 - 4y_i(\Delta+1)(n-\Delta-1)}}{(\Delta+1)(n-\Delta-1)}$$

where $x_i = 2(n - \overline{Tr}_i - 1)\Delta^2 + 2(W - \overline{Tr}_i - 1)\Delta + 2W$ and $y_i = \Delta^2(4W - \overline{Tr}_i^2 - 2\overline{Tr}_i - 1)$ and $\overline{Tr}_i$ denotes the average distance degree of the vertex v_i;

(ii) if $\Delta = n-1$, then

$$s_D = \begin{cases} 0 & \text{if} \quad n = 1, \\ 2 & \text{if} \quad n = 2, \\ n + \sqrt{n^2 - 3n + 3} & \text{if} \quad n \geq 3. \end{cases}$$

For the particular case of graphs on n vertices with a given clique number ω, Yu et al. [145] proved the following bounds.

Theorem 6.2 ([145]) *Let G be a graph on n vertices with a clique number ω and Wiener index W. Suppose that $G_1, G_2, \ldots, G_k$ are all the cliques of G of order ω. For $1 \leq i \leq k$, let $W_i = \sum_{v_j \in G_i} Tr_j$ and $\overline{W}_i = \sum_{v_j \notin G_i} Tr_j$. We have:*

(i) if $\omega = n$, then $s_D(G) = n$;

(ii) if $\omega \le n-1$*, then*

$$s_D(G) \ge \max_{1\le i\le k} \frac{\sqrt{x_i^2 - 4y_i^2\omega(n-\omega)}}{\omega(n-\omega)}$$

where $x_i = \omega(\overline{W}_i - W_i + n(\omega-1))$ *and* $y_i = 2W\omega(\omega-1) - W_i^2$.

Using the above theorem, Yu et al. [145] deduced the next result (stated using the same notation).

Corollary 6.3 ([145]) *Let* G *be a graph on* n *vertices with clique number* $\omega \le n-1$*. Then*

$$\partial_1(G) \ge \max_{1\le i\le k} \frac{x_i + \sqrt{x_i^2 - 4y_i^2\omega(n-\omega)}}{2\omega(n-\omega)} \qquad \text{and} \qquad \partial_n(G) \le \max_{1\le i\le k} \frac{x_i - \sqrt{x_i^2 - 4y_i^2\omega(n-\omega)}}{2\omega(n-\omega)}.$$

The bounds given in Theorem 6.1 and 6.2 are not sharp, but Yu et al. [145] provided sharp bounds under different conditions. First, the next result is a lower on the distance spectral spread over all graphs with given order.

Theorem 6.4 ([145]) *Let* G *be a graph on* n *vertices. Then* $s_D(G) \ge n$ *with equality if and only if* G *is the complete graph* K_n.

For the case of bipartite graphs, we have

Theorem 6.5 ([145]) *Let* G *be a bipartite graph on* n *vertices. Then*

$$s_D(G) \ge \sqrt{\left\lfloor \frac{n}{2} \right\rfloor^2 - \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil + \left\lceil \frac{n}{2} \right\rceil^2}$$

with equality if and only if G *is the complete bipartite graph* $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$

For the class of trees on n vertices, the bound is the following.

Theorem 6.6 ([145]) *Let* T *be a tree on* n *vertices. Then*

$$s_D(T) \ge n + \sqrt{n^2 - 3n + 3}$$

with equality if and only if T *is the star* S_n.

Finally, a lower bound on the class of graphs with given order n and independence number α.

Theorem 6.7 ([145]) *Let* G *be a graph on* $n \ge 2$ *vertices with independence number* $\alpha \ge 2$*. Then*

$$s_D(G) \ge \frac{n + \alpha + 1 + \sqrt{(n-\alpha+1)^2 + 2\alpha(\alpha-1)}}{2}$$

with equality if and only if G *is the complete split graph* $CS(n, n-\alpha)$.

7 Other distance eigenvalues and frequencies

In this section, we report on the results related to the distance eigenvalues of a connected graph, other that the largest eigenvalue. We also report about results related to the frequencies of the distances eigenvalues. Note that those topics attracted the attention of the researchers less than the spectral radius or the characteristic polynomial did.

In a recent paper, Yu [142] studied some classes of graph that are characterized by their lest distance eigenvalue ∂_n.

Theorem 7.1 ([142]) *Let* G *be a graph on* n *vertices with least distance eigenvalue* ∂_n*. Then we have*

(a) $\partial_n = 0$ *if and only if* $G \cong K_1$*;*

(b) *for* $n \geq 2$, $\partial_n = -1$ *if and only if* $G \cong K_n$;

(c) *for* $n \geq 3$, $\partial_n = -2$ *if and only if* $G \cong K_{n_1,n_2,\ldots,n_s}$ *for some* $2 \leq s \leq n-1$ *with* $n_1 + n_2 + \ldots + n_s = n$;

(d) *for* $n \geq 3$, *if* $G \ncong K_n$ *and* $G \ncong K_{n_1,n_2,\ldots,n_s}$ *for some* $2 \leq s \leq n-1$ *with* $n_1 + n_2 + \ldots + n_s = n$, $\partial_n < -2.383$.

In the same paper [142], the author also stated analogous results for the class of bipartite graphs and for the class of trees. Regarding the bipartite graphs the differences are that in part (b) the only complete graph that is bipartite is K_2; in part (c) s must be 2; and finally in part (d) we have $\partial_n < -3.414$ instead of $\partial_n < -2.383$. Thereafter, for the class of trees compared to bipartite graphs, the only difference is in part (c) in the theorem, since the only complete bipartite graph which is also a tree is the star S_n.

As a consequence of the above results the following corollary.

Corollary 7.2 ([142])

(i) *There exists no graph with* $\partial_n \geq -2.383$ *and* $\partial_n \notin \{-2, -1, 0\}$.

(ii) *There exists no bipartite graph with* $\partial_n \geq -3.414$ *and* $\partial_n \notin \{-2, -1, 0\}$.

Using his computer program Graffiti, designed for conjecture making in graph theory, Fajtlowicz [57] generated a series of conjectures relating graph invariants. In some of these conjectures the distance eigenvalues and/or their frequencies in the distance spectrum were involved. We next list and comment some of those conjectures.

The first conjecture we list is an inequality between the largest negative distance eigenvalue and the matching number of a connected graph.

Conjecture 7.3 (WOW-32 in [57]) *For a connected graph* G, $-\max\{\partial_i : \partial_i < 0\} \leq \mu$, *where* μ *denotes the matching number of* G.

As far as we known, the above conjectures remains open. Experiments using the AutoGraphiX system (a software devoted to conjecture–making in graph theory, see [2, 3, 31, 33]) confirm the above conjecture and suggest that the extremal graphs are the complete bipartite $K_{n-2,2}$, $n \geq 4$. For $n = 8$, AutoGraphiX found two graphs $K_{6,2}$ and the cube graph Q_3.

The next Graffiti conjectures is an inequality between the largest negative distance eigenvalue and the diameter of a connected graph.

Conjecture 7.4 (WOW-35 in [57]) *For a connected graph* G, $D \leq -\max\{\partial_i : \partial_i < 0\}$, *where* D *denotes the diameter of* G.

It is mentioned in [57] that the above conjecture was proved by James B. Shearer (no reference provided), however there is certainly a mistake. Indeed, as stated the conjecture is not true and there are so many families of graphs for which it does not hold. Even if we reverse the inequality the result is not true since for any integer $p \geq 4$, the graph $K_{p,p} - M$, where M is a perfect matching, is a counterexample. Also, the cube graphs Q_p are counterexamples for $p \geq 3$.

Along these lines, we compared the diameter D with the negative of the least distance eigenvalue and get the following conjecture.

Conjecture 7.5 *For a connected graph* G, $D \leq -\partial_n$, *where* D *denotes the diameter of* G. *Equality holds if and only if* G *is a multipartite graph.*

The inequality in the above conjecture is true. Indeed, the leat eigenvalue is the minimum of the Rayleigh quotient, *i.e.*,

$$\partial_n = \min_{X \neq 0} \frac{X^T \mathcal{D} X}{X^T X}.$$

If we consider the vector X with $X_i = 1$ and $X_j = -1$ for for two vertices i and j such that $d(i,j) = D$, and $X_k = 0$ for $k \neq i, j$, then the quotient equals $-D$ and the inequality follows.

The above statement is the best we can conjecture since there exist graphs with $D \leq -\partial_{n-1}$ and others with $D \geq -\partial_{n-1}$. For instance, the path P_n satisfies $D \geq -\partial_{n-1}$ for $n \leq 14$ and $D \leq -\partial_{n-1}$ for $n \geq 15$.

Conjecture 7.6 (WOW-313 in [57]) *For a connected triangle free graph G, $m/\alpha \leq p_-(\mathcal{D})$, where m, α and $p_-(\mathcal{D})$ denote respectively the size, the independence number and the number of positive distance eigenvalues of G.*

Experiments with AutoGraphiX confirm the above conjectures. It seems that equality holds only when n is even, in which case, the extremal graphs are $K_{\frac{n}{2},\frac{n}{2}} - M$, where M is a perfect matching for $n \geq 8$.

Conjecture 7.7 (WOW-404 in [57]) *For a connected graph G, with independence number $\alpha \leq 2$, $\partial_2 \leq tr$, where tr denotes the number of triangles in G.*

This conjecture was confirmed with AutoGraphiX and the gap between tr and ∂_2 is arbitrarily large. Indeed, in the case of an even number of vertices $n = 2p$ with $p \geq 3$, the experiments suggest that the extremal graph is the Cartesian product of a clique K_p and K_2 denoted $K_p \Box K_2$ (see Figure 52 for $K_5 \Box K_2$), for which $\partial_2 = 0$ (see Corollary 4.6) and $tr = p(p-1)(p-2)/3 = n(n-2)(n-4)/24$.

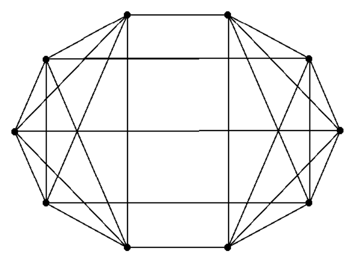

Figure 52: The graph $K_5 \Box K_2$.

We list some proved Graffiti conjectures related to the distance spectrum.

The *temperature* of a vertex v in a graph G is defined as $Tp(v) = d(v)/(n - d(v)$, where $d(v)$ denote the degree of v. The *average temperature* in a graph G is denote by $\overline{Tp} = \overline{Tp}(G)$.

Theorem 7.8 (WOW-25 in [57]) *Let G be a connected graph on $n \geq 2$ vertices with average temperature $\overline{Tp}$ and distance matrix $\mathcal{D}$. Then $\overline{Tp} \leq p_-(\mathcal{D})$, where $p_-(\mathcal{D})$ denotes the number of negative distance eigenvalues.*

As mentioned in [57], the above result is by Shearer. The extremal graphs for the above conjecture seem to be only the complete graphs.

Conjecture 7.9 (WOW-36 in [57]) *For a connected graph G, $D \leq p_-(\mathcal{D})$, where D denotes the diameter of G.*

The paths are among the extremal graphs for the above conjecture, and among the trees they are the only extremal trees. Indeed, the path P_n is the only tree (graph) with diameter $D = n - 1$, and according to Corollary 2.3, the path P_n has exactly $n - 1$ negative distance eigenvalues.

The *dual degree* $d^*(v)$ of a vertex v is the average degree of its neighbors. The minimum dual degree in a graph is denoted by δ^*. The *girth* $g = g(G)$ of a graph G is the length of a smallest cycle in G, if any.

Conjecture 7.10 (WOW-284 in [57]) *Let G be a connected graph on $n \geq 3$ vertices with girth $g \geq 5$ and minimum dual degree δ^*. Then $\delta^* \leq -\partial_n$, where ∂_n denote the least distance eigenvalue of G.*

As far as we know, the above conjecture remains open. The Petersen graph is among the graphs for which $\delta^* = -\partial_n$ $(= 3)$ and $g = 5$.

Finally, we list some refuted Graffiti conjectures related to the distance spectrum.

The *Randić index* $Ra = Ra(G)$of a graph $G = (V, E)$ is defined by

$$Ra = Ra(G) = \sum_{uv \in E} \frac{1}{d(u) \cdot d(v)}$$

where $d(u)$ denotes the degree of u in G.

Conjecture 7.11 (WOW-29 in [57]) *Let G be a connected graph on $n \geq 2$ vertices with Randić index Ra. Then $Ra \leq p_-(\mathcal{D})$.*

Counterexamples for the above conjecture with 9 and 10 vertices are illustrated in Figure 53.

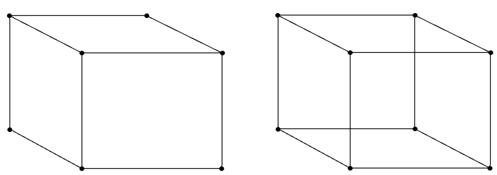

Figure 53: Counterexamples for Conjecture 7.11 and 7.14

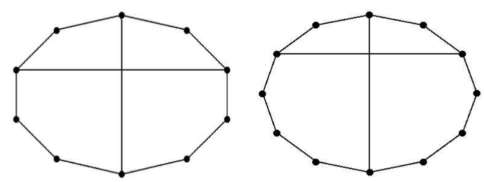

Figure 54: Counterexamples for Conjecture 7.12

Conjecture 7.12 (WOW-30 in [57]) *Let $G = (V, E)$ be a connected graph on $n \geq 2$. Then*

$$p_+(\mathcal{D}) \leq \sum_{v \in V} Tp(v).$$

Counterexamples for the above conjecture with 10 and 12 vertices are illustrated in Figure 54.

Conjecture 7.13 (WOW-31 in [57]) *Let G be a connected graph on $n \geq 2$ vertices with independence number α and distance spectrum $\partial_1, \partial_2, \ldots, \partial_n$. Then $\alpha \geq -\max\{\partial_i : \partial_i < 0\}$.*

The complement of the Petersen graph, which is also the line graph of the complete graph K_5, is a counterexample for the above conjecture.

Conjecture 7.14 (WOW-33 in [57]) *Let G be a connected graph on $n \geq 2$ vertices with chromatic number χ and distance spectrum $\partial_1, \partial_2, \ldots, \partial_n$. Then $\chi \geq -\max\{\partial_i : \partial_i < 0\}$.*

Conjecture 7.15 (WOW-166 in [57]) *Let G be a connected graph on $n \geq 2$ vertices and m edges. Then $\sqrt{m} \leq p_-(\mathcal{D}) + p_0(\mathcal{D})$.*

Conjecture 7.15 was refuted in [24] and three counterexamples on 9 are illustrated in Figure 55, where the sign + means add an edge between each vertex on the right and each vertex on the left.

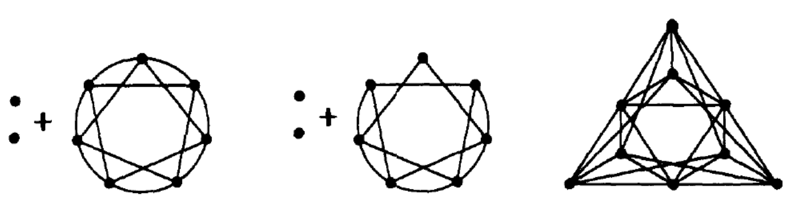

Figure 55: Counterexamples for Conjecture 7.15 on 9 vertices.

The *energy* $En = En(G)$ of a graph is the sum of the absolute values of the adjacency eigenvalues of G, *i.e.*, $En = En(G) = \sum_{i=1}^{n} |\lambda_i|$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ denote the adjacency eigenvalues of G.

Conjecture 7.16 (WOW-48 in [57]) *Let G be a connected regular graph on $n \geq 2$ vertices with energy En. Then $En \leq 2\partial_1$.*

A counterexample for the above conjecture is the complement of the graph on 15 vertices composed of the Petersen graph together with 5 isolated vertices.

Conjecture 7.17 (WOW-281 in [57]) *Let G be a connected graph on $n \geq 3$ vertices. Then $\max\{\mu, \overline{\mu}\} \leq p_-(\mathcal{D})$, where μ and $\overline{\mu}$ denote the matching number in G and $\overline{G}$, respectively, and $p_-(\mathcal{D})$ denotes the number of negative distance eigenvalues of G.*

In Figure 56 are illustrated two counterexamples for Conjecture 7.17 on 8 and 10 vertices.

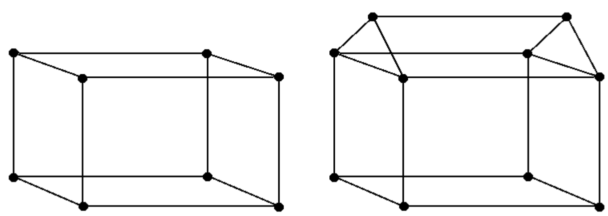

Figure 56: Counterexamples for Conjecture 7.17 on 8 and 10 vertices.

Conjecture 7.18 (WOW-283 in [57]) *Let G be a connected graph on $n \geq 3$ vertices and $m \geq n$ edges with girth $g \geq 5$. Then $\alpha \leq p_-(\mathcal{D}) + p_0(\mathcal{D})$, where α, $p_-(\mathcal{D})$ and $p_0(\mathcal{D})$ denote respectively the independence number, the number of negative distance eigenvalues and the multiplicity of 0 as an eigenvalue of G.*

Conjecture 7.19 (WOW-405 in [57]) *Let G be a connected graph on $n \geq 3$ vertices with independence number $\alpha \leq 2$. Then $-\partial_n \leq \mu + \overline{\mu}$, where μ and $\overline{\mu}$ denote the matching number in G and $\overline{G}$, respectively, and ∂_n denotes the least distance eigenvalue of G.*

The above conjectures was first disproved in [50]. Figure 57 shows counterexamples on 7 and 8 vertices.

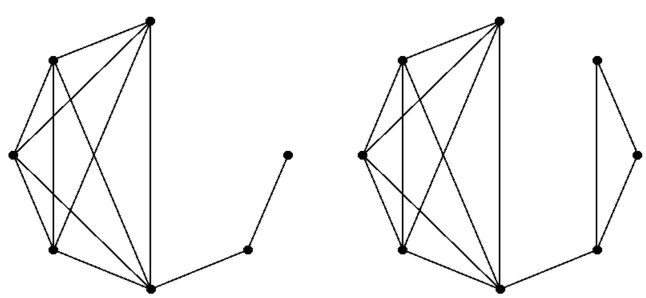

Figure 57: Counterexamples for Conjecture 7.19

8 The distance energy

Introduced by Indulal, Gutman and Vijayakumar [85], the *distance energy* of a graph G is defined as the sum of the absolute values of its distance eigenvalues, *i.e.*,

$$E_D(G) = \sum_{i=1}^{n} |\partial_i(G)|.$$

Most of theorems given in Section 4 can be used to calculate the distance energy of some particular graphs. In [84], the authors computed the distance energy of

- the double graph of an even cycle from Theorem 4.4: $E_D(D_2C_{2k}) = 4k(k+1)$;
- the corona of the cycle from Theorem 4.8:

$$E_D\left(Cor(C_n)\right) = \begin{cases} 2\left((n-1)^2 + \sqrt{(n-1)^4 + 6n^2}\right) & \text{if } n \text{ is even} \\ 2\left(n(n+3) + \sqrt{n^2(n+3)^2 + 6n(n+1) + 1}\right) & \text{if } n \text{ is odd;} \end{cases}$$

- the Cartesian product of any graph G on p vertices with K_2 from Theorem 4.5: $E_D(G \Box K_2) = 2(E_D(G) + p)$;
- the composition of the even cycle C_{2k} with K_2 from Theorem 4.7: $E_D(C_{2k} \circ K_2) = 2k(2k+1)$;
- the extended double cover of $C_p \nabla C_p$ from Theorem 4.10:

$$E_D(EDC(C_p \nabla C_p)) = \begin{cases} 40 & \text{if} \quad p = 3, \\ 4(E(C_p) + 5p - 10) & \text{if} \quad p \geq 4, \end{cases}$$

  where $E(C_p)$ denotes the adjacency energy of C_p.

Since the diagonal entries of the distance matrix are 0's, the sum of all the distance eigenvalues of a graph is 0, *i.e.*, $\partial_1 + \partial_2 + \cdots + \partial_n = 0$. Thus, we have

$$E_D(G) = \sum_{i=1}^{n} |\partial_i(G)| = 2 \sum_{\partial_i > 0} \partial_i(G) = 2 \sum_{\partial_i < 0} |\partial_i(G)|.$$

As an immediate consequence of the above relation, $E_D(G) \geq 2\partial_1$, and therefore any lower bound on ∂_1 is also a lower bound on $E_D(G)/2$. This fact is more important for the class of graphs with only one positive distance eigenvalue such as trees. Indeed, for such a graph G, $E_D(G) = 2\partial_1(G)$. Using this fact and a lower bound on ∂_1 proved by Das [46], Zhou and Ilić [151] stated the following theorem.

Theorem 8.1 ([151]) *Let G be a graph on $n \geq 2$ vertices. Then*

$$E_D(G) \geq 2\sqrt{\frac{1}{n}\sum_{i=1}^{n} Tr_i^2}$$

with equality if and only if G a transmission regular graph wit exactly one positive distance eigenvalue.

In the same paper [151] and again using bounds on ∂_1, the authors provided lower bounds on E_D: one in terms of the order and the Wiener index of G, and another in terms of the order and the size of G.

Theorem 8.2 ([151]) *Let G be a graph on $n \geq 2$ vertices and m edges with Wiener index W. Then*

$$E_D(G) \geq \frac{4W}{n}$$

with equality if and only if G a transmission regular graph wit exactly one positive distance eigenvalue. Moreover,

$$E_D(G) \geq 4(n-1) - \frac{4m}{n}$$

with equality if and only if either $G \cong K_n$ or G is a (transmission) regular graph of diameter two with exactly one positive distance eigenvalue.

Note that the second bound in Theorem 8.2 was conjectured in [32].

In 2008, Ramane et al. [110] conjectured that among graphs on n vertices, the complete graph K_n minimizes the distance energy. In virtue of Theorem 8.2, the conjecture is true.

Ramane et al. [110] proved a series of upper and lower bounds on the distance energy of a graph on n vertices. These bounds are given in the next three theorems.

Theorem 8.3 ([110]) *Let G be a graph on n vertices and m edges. Then*

$$\sqrt{2M + n(n-1)|det(\mathcal{D})|^{\frac{2}{n}}} \leq E_D(G) \leq \sqrt{2Mn},$$

where $M = 2n(n-1) - 3m$.

In virtue of Graham's result, Theorem 2.1, in the case of a tree T, the bounds in the above theorem depends only on the order n of T, *i.e.*

$$\sqrt{(4n-6)(n-1) + 4n(n-1)\left(\frac{n-1}{4}\right)^{\frac{2}{n}}} \leq E_D(T) \leq \sqrt{(4n-6)n(n-1)}.$$

The next theorem provides a lower and an upper bounds depending only on the order n and size m of G.

Theorem 8.4 ([110]) *Let G be a graph on n vertices and m edges. Then*

$$2\sqrt{M} \leq E_D(G) \leq \sqrt{M\left(1 + \sqrt{1 + 8M}\right)},$$

where $M = 2n(n-1) - 3m$.

The last theorem in [110] gives a lower and an upper bounds on E_D in terms of the order n only.

Theorem 8.5 ([110]) *Let G be a graph on n vertices and m edges. Then*

$$\sqrt{n(n-1)} \leq E_D(G) \leq \sqrt{\frac{n^3(n^2-1)}{6}}.$$

Romane et al. [111] proved a series of lower and upper bounds on the distance energy using the sum of the squares of the distances in addition to the order.

Theorem 8.6 ([111]) *Let G be a graph on n vertices. Then*

$$\sqrt{2\sum_{1\leq i<j\leq n}(d_{ij})^2 + n(n-1)|det(\mathcal{D})|^{\frac{2}{n}}} \leq E_D(G) \leq \sqrt{2n\sum_{1\leq i<j\leq n}(d_{ij})^2}.$$

The upper bound in the above Theorem 8.6 was improved by Bozkurt, Güngör and Zhou [23].

Theorem 8.7 ([23]) *Let G be a graph on n vertices. Then*

$$E_D(G) \leq \sqrt{2(n-1)\sum_{1\leq i<j\leq n}(d_{ij})^2 + n|det(\mathcal{D})|^{\frac{2}{n}}}.$$

Note that the bounds corresponding to those of Theorem 8.6 and Theorem 8.7 for the case of trees, obtained using Theorem 2.1, were given in [111] and [23], respectively.

Another upper bound on E_D was proved by Ramane et al. [111].

Theorem 8.8 ([111]) *Let G be a graph on n vertices and m edges. Then*

$$E_D(G) \leq \frac{2}{n}\sum_{1\leq i<j\leq n}(d_{ij})^2 + \sqrt{(n-1)\left[2\sum_{1\leq i<j\leq n}(d_{ij})^2 - \left(\frac{2}{n}\sum_{1\leq i<j\leq n}(d_{ij})^2\right)^2\right]}.$$

For the case of graphs of diameter 2, the next corollary follows from Theorem 8.8.

Corollary 8.9 ([111]) *Let G be a graph on n vertices and m edges with diameter at most 2. Then*

$$E_D(G) \leq \frac{4n(n-1)-6m}{n} + \sqrt{(n-1)\left[4n(n-1)-6m-\left(\frac{4n(n-1)-6m}{n}\right)^2\right]}.$$

Using the transmission and the second distance degree sequences, Indulal [82] proved a sharp upper bound on the distance energy $E_D(G)$ of a graph G.

Theorem 8.10 ([82]) *Let G be a graph on n vertices with distance energy $E_D(G)$ and transmission and second distance degree sequences $\{Tr_1, Tr_2, \ldots, Tr_n\}$ and $\{Tr_1^{(2)}, Tr_2^{(2)}, \ldots, Tr_n^{(2)}\}$ respectively. Then*

$$E_D(G) \leq \sqrt{\frac{\sum_{i=1}^n (Tr_i^{(2)})^2}{\sum_{i=1}^n Tr_i^2}} + \sqrt{(n-1)\left(2S - \frac{\sum_{i=1}^n (Tr_i^{(2)})^2}{\sum_{i=1}^n Tr_i^2}\right)},$$

where S denotes the sum of the squares of all the distances between all unordered pairs of vertices of G. Equality holds if and only if G is the complete graph or a pseudo k–distance regular graph with three distinct eigenvalues k, $\sqrt{\frac{S-k^2}{n-1}}$ and $-\sqrt{\frac{S-k^2}{n-1}}$.

Similarly to the generalization of Theorem 5.9 to Theorem 5.10, Güngör and Bozkurt [67] generalized the above theorem.

Theorem 8.11 ([67]) *Let G be a graph on n vertices, t be a real number and k be an integer. Then*

$$E_D(G) \leq \sqrt{\frac{\sum_{i=1}^n \left(M_i^{(k+1)}\right)^2}{\sum_{i=1}^n \left(M_i^{(k)}\right)^2}} + \sqrt{(n-1)\left(2S - \frac{\sum_{i=1}^n \left(M_i^{(k+1)}\right)^2}{\sum_{i=1}^n \left(M_i^{(k)}\right)^2}\right)},$$

where S denotes the sum of the squares of all the distances between all unordered pairs of vertices of G. Equality holds if and only if G is the complete graph or a graph satisfying

$$\frac{M_1^{(k+1)}}{M_1^{(k)}} = \frac{M_2^{(k+1)}}{M_2^{(k)}} = \cdots = \frac{M_n^{(k+1)}}{M_n^{(k)}} = \ell \geq \frac{2S}{n}$$

with three distinct eigenvalues ℓ, $\sqrt{\frac{S-k^2}{n-1}}$ and $-\sqrt{\frac{S-k^2}{n-1}}$.

Caporossi, Chasset and Furtula [32], after experiments using the AutoGraphiX system (a software devoted to conjecture–making in graph theory, see [2, 3, 31, 33]), suggested the following conjecture. Before stating the conjecture, we need to recall the definition of the *Soltés* graph [128]. Let u be an isolated vertex or one end vertex of a path. Let us join u with at least one vertex of a complete graph. The graph so obtained is the *Soltés graph* $PK_{n,m}$, also called the *path–complete* graph, where n is its order and m its size. There is exactly one $PK_{n,m}$ for given n and m such that $1 \leq n-1 \leq m \leq n(n-1)/2$. Among all graphs with given order n and size m, $PK_{n,m}$ maximizes (non uniquely) the diameter [70] and (uniquely) the average distance [128].

Conjecture 8.12 ([32]) *Among all graphs of order n and size m with $n \leq m \leq (n-2)(n-3)/2$, the path–complete graph $PK_{n,m}$ maximizes the distance energy.*

Now, we turn to the survey of the results about bounding the distance energy over the class of graphs with diameter 2. First, we give lower and upper bounds on $E_D(G)$ in terms of order n and size m of G.

Theorem 8.13 ([85]) *Let G be a graph on n vertices and m edges of diameter 2. Then*

$$\sqrt{4n(n-1)-6m+n(n-1)|det(\mathcal{D})|^{\frac{2}{n}}} \leq E_D(G) \leq \sqrt{2n\left(2n^2-3m-2n\right)}.$$

Note that Theorem 8.13 can be obtained as a corollary from Theorem 8.3 or from Theorem 8.6.

Another upper bound in terms of the order n and size m is the following.

Theorem 8.14 ([85]) *Let G be a graph on n vertices and m edges with diameter 2. Then*

$$E_D \leq \frac{1}{n}\left(2n^2 - 2m - 2n + \sqrt{(n-1)\left((2n+m)(2n^2-4m) - 4n^2\right)}\right)$$

In addition to have diameter 2, the graphs in the next result are assumed to be degree regular.

Theorem 8.15 ([85]) *Let G be a k–regular graph on n vertices with diameter 2. Then*

$$E_d(G) \leq 2n - k - 2 + \sqrt{(n-1)\left(n(k+4) - (k+2)^2\right)}$$

Note that over the class of diameter 2, *degree regular* is equivalent to *transmission regular*.

The following result follows form Theorem 2.18 using the fact that if a graph has exactly one positive distance eigenvalue ∂_1 then its distance energy is $E_D = 2\partial_1$.

Theorem 8.16 ([112]) *If G is a k–regular graph on n vertices with diameter $D \leq 2$ such that none of the graph F_1, F_2 and F_3 (Figure 58) is an induced subgraph of G, then the $\mathcal{D}$–energy of $L(G)$ is*

$$E_D(L(G)) = 2k(n-2).$$

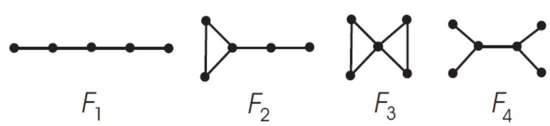

Figure 58: Some forbidden graphs.

The next corollary follows from and generalizes, in some way, the above theorem.

Corollary 8.17 ([112]) *Let G be a k–regular graph on n vertices with diameter $D \leq 2$ and let none of the four graphs of Figure 58 be an induced subgraph of G. Let n_p and k_p be the order and degree, respectively, of the p–th iterated line graph $L^p(G)$ of G, $p \geq 1$. Then the $\mathcal{D}$–energy of $L^p(G)$ is*

$$E_D(L^p(G)) = 2n_{p-1}k_{p-1} - 4k_{p-1} = 4n_p - 2k_p - 4 = 4n\prod_{i=1}^{p-1}(2^{i-1}k - 2^i + 1) - 2(2^pk - 2^{p+1} + 4).$$

Zhou and Ilić [151] proved an upper bound on the distance energy of a graph G of diameter 2 using the adjacency energy $E(\overline{G})$ of its complement $\overline{G}$.

Theorem 8.18 ([151]) *Let G be a graph on n vertices with diameter at most 2. Then*

$$E_D(G) \leq 2(n-1) + E(\overline{G}),$$

where $E(\overline{G})$ denotes the (adjacency) energy og $\overline{G}$, the complement of G.

Two graphs G_1 and G_2 are said to be *distance equienergetic* or $\mathcal{D}$*–equienergetic* if they have the distance energy, *i.e.*, $E_(G_1) = E_D(G_2)$. Evidently, two distance cospectral, or $\mathcal{D}$–cospectral graphs are $\mathcal{D}$–equienergetic. Thus the study of $\mathcal{D}$–equienergetic focusses on non $\mathcal{D}$–cospectral graphs. Several authors were interested in the problem of finding $\mathcal{D}$–equienergetic but non $\mathcal{D}$–cospectral graphs. Some infinite families of such graphs were constructed.

In order to construct $\mathcal{D}$–equienergetic but non $\mathcal{D}$–cospectral graphs, Ramane et al. [112] proved the following lemma.

Lemma 8.19 ([112]) *Let G_1 and G_2 be two k–regular graphs on n vertices each, with diameters $D_1, D_2 \leq 2$. Assume that none of the four graphs of Figure 58 is an induced subgraph of G_i, $i = 1, 2$. Then for any $p \geq 1$, the following holds:*

- *$L^p(G_1)$ and $L^p(G_2)$ are of the same order, same degree and have the same number of edges.*
- *$L^p(G_1)$ and $L^p(G_2)$ are $\mathcal{D}$–cospectral if and only if G_1 and G_2 are cospectral.*

Using Corollary 8.17 and Lemma 8.19, Ramane et al. [112] deduced the next theorem which a way for constructing $\mathcal{D}$–equienergetic but non $\mathcal{D}$–cospectral graphs.

Theorem 8.20 ([112]) *Let G_1 and G_2 be two k–regular graphs on n vertices each, with diameters $D_1, D_2 \leq 2$. Assume that none of the four graphs of Figure 58 is an induced subgraph of G_i, $i = 1, 2$. Then for any $p \geq 1$, the iterated line graphs $L^p(G_1)$ and $L^p(G_2)$ form a pair of non $\mathcal{D}$–cospectral, $\mathcal{D}$–equienergetic graphs of equal order and of equal number of edges.*

Ramane, Gutman and Revankar [109] computed the distance energy of the join of two regular graphs with diameters at most 2.

Theorem 8.21 ([109]) *For $i = 1, 2$, let G_i be a k_i–regular graph on n_i vertices, with respective diameters $D_1, D_2 \leq 2$. For $i = 1, 2$, let $t_i = 2n_i - k_i - 2$. Then*

$$E_D(G_1 \nabla G_2) = \begin{cases} E_D(G_1) + E_D(G_2) & \text{if } t_1 t_2 \geq n_1 n_2 \\ E_D(G_1) + E_D(G_2) - (t_1 + t_2) + \sqrt{(t_1 + t_2)^2 - 4(t_1 t_2 - n_1 n_2)} & \text{if } t_1 t_2 < n_1 n_2. \end{cases}$$

The authors of the above theorem used it to construct an infinite family of $\mathcal{D}$–equienergetic but non $\mathcal{D}$–cospectral graphs.

Stevanović and Indulal [132] computed the distance energy of the join of two regular graphs whose smallest eigenvalue is at least -2.

Theorem 8.22 ([132]) *For $i = 1, 2$, let G_i be a k_i–regular graph on n_i vertices, whose smallest eigenvalue of the adjacency matrix is at least -2 and such that $G_i \ncong K_n$. Then*

$$E_D((G_1 \nabla G_2) = 4(n_1 + n_2) - 2(k_1 + k_2) - 8.$$

Using the above result and Theorem 4.12, Stevanović and Indulal [132] constructed an infinite family of sets of $\mathcal{D}$–equienergetic but non $\mathcal{D}$–cospectral graphs. For a fixed integer n, let $\mathcal{P}_n$ the set of integer partitions of n into parts of size at least three. For $P = \{p_1, p_2, \ldots, p_k\} \in \mathcal{P}_n$, we denote $\mathcal{C}_P$ the union of cycles of sizes $p_1, p_2, \ldots, p_k$.

Corollary 8.23 ([132]) *Let G be a k–regular graph. Then, the graphs $K_1 \nabla (\mathcal{C}_P \cup G)$, $P \in \mathcal{P}_n$, are $\mathcal{D}$–equienergetic but non $\mathcal{D}$–cospectral.*

Using Theorem 4.13, Stevanović [129] deduced a method for constructing an infinite family of pairs of $\mathcal{D}$–equienergetic but non $\mathcal{D}$–cospectral graphs. This construction uses joined union of regular graphs.

Theorem 8.24 ([129]) *Let G be a graph with vertex set $V = \{v_1, v_2, \ldots, v_n$, and for $i = 1, 2, \ldots, n$, let G_i and H_i be k_i–regular graphs of order n_i whose smallest adjacency eigenvalue is at least -2. Then $E_D(G[G_1, G_2, \ldots G_n]) = E_D(G[H_1, H_2, \ldots H_n])$.*

Indulal and Gutman [84] constructed an infinite family of pairs of $\mathcal{D}$–equienergetic non $\mathcal{D}$–cospectral bipartite graphs from pairs of non A–cospectral cubic graphs.

Theorem 8.25 ([84]) *Let G_1 and G_2 be two cubic non A–cospectral graphs $2n$ vertices each. Then the extended double cover graphs $EDC(L^2(G_1) \nabla L^2(G_1))$ and $EDC(L^2(G_1) \nabla L^2(G_1))$ are $\mathcal{D}$–equienergetic but non $\mathcal{D}$–cospectral graphs on $24n$ vertices each.*

After computing the $\mathcal{D}$–energy of complete bipartite graphs, Liu [97] showed that for any three integers n, a and b such that $n-b \geq b > a \geq 2$, the two complete bipartite graphs $K_{a,n-a}$ and $K_{b,n-b}$ are $\mathcal{D}$–equienergetic but non $\mathcal{D}$–cospectral. In the same paper [97], it was also shown that for any integer $p \geq 4$, the two graphs $K_{p,p}$ and $K_{p,p} - M$, where M is a perfect matching, are $\mathcal{D}$–equienergetic but non $\mathcal{D}$–cospectral.

Ilić, Bašić and Gutman [79] constructed a family of pairs of integral circulant graphs equienergetic but non cospectral with respect to the adjacency, Laplacian and distance spectra simultaneously.

To end this section, and therefore the present paper, we give a Nordhaus–Gaddum type inequality for the distance energy of a graph and its complement. It is proved by Zhou and Ilić [151].

Theorem 8.26 ([151]) *Let G be a graph on $n \geq 4$ vertices with a connected complement $\overline{G}$. Then*

$$E_D(G) + E_D(\overline{G}) \geq 6(n-1)$$

with equality if and only if G and $\overline{G}$ are both regular graphs of diameter two and both have exactly one positive distance eigenvalue.

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