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D-EQUIENERGETIC SELF-COMPLEMENTARY GRAPHS

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Abstract. The D-eigenvalues $\{\mu_1, \mu_2, \ldots, \mu_n\}$ of a graph G are the eigenvalues of its distance matrix D and form the D-spectrum of G denoted by $spec_D(G)$. The D-energy $E_D(G)$ of the graph G is the sum of the absolute values of its D-eigenvalues. We describe here the distance spectrum of some self-complementary graphs in the terms of their adjacency spectrum. These results are used to show that there exists D-equienergetic self-complementary graphs of order $n = 48t$ and $24(2t+1)$ for $t \geq 4$.

1. INTRODUCTION

Let G be a simple graph on n vertices and let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of its adjacency matrix A. The energy of a graph is defined as

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| \ .$$

For details on this currently much studied graph–spectral invariant see [4, 5, 6]. After the introduction of the analogous concept of Laplacian energy [7], it was recognized [1] that other energy-like invariants can be defined as well, among them the *distance energy*.

Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$. The distance matrix $D = D(G)$ of G is defined so that its (i,j)-entry d_{ij} is equal to $d_G(v_i, v_j)$, the distance between the vertices v_i and v_j of G. The eigenvalues of $D(G)$ are said to be the D-eigenvalues of G and form the D-spectrum of G, denoted by $spec_D(G)$. Since the distance matrix is symmetric, all its eigenvalues μ_i , $i = 1, 2, \dots, n$, are real and can be labelled so that $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$.

The D-energy, $E_D(G)$, of G is then defined as

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

The concept of D-energy, Eq. (1), is recently introduced [11]. This definition was motivated by the much older and nowadays extensively studied graph energy. This invariant was studied by Consonni and Todeschini [1] for possible use in QSPR modelling. Their study showed, among others, that the distance energy is a useful molecular descriptor, since the values of $E_D(G)$ or $E_D(G)/n$ appear among the best univariate models for the motor octane number of the octane isomers and for the water solubility of polychlorobiphenyls. For some recent works on D-spectrum and D-energy of graphs see [8, 9, 10, 11, 13].

Two graphs with equal D-energy are said to be D-equienergetic. D-cospectral graphs are evidently D-equienergetic. Therefore, in what follows we focus our attention to D-equienergetic non$-D$-cospectral graphs. In this paper we search for self-complementary graphs of this kind. A similar work on pairs of ordinary equienergetic self-complementary graphs is [12].

All graphs considered in this paper are simple and we follow [2] for spectral graph theoretic terminology. We shall need:

Lemma 1. [2] *Let G be an r-regular connected graph, with*

$spec(G) = \{r, \lambda_2, \ldots, \lambda_n\}$. *Then*

$$spec(L^2(G)) = \begin{pmatrix} 4r-6 & \lambda_2+3r-6 & \cdots & \lambda_n+3r-6 & 2r-6 & -2 \\ 1 & 1 & \cdots & 1 & \frac{n(r-2)}{2} & \frac{nr(r-2)}{2} \end{pmatrix}.$$

Let G be a graph. Then the following construction [3] results in a self-complementary graph $\mathcal{H}$. Recall that a graph $\mathcal{H}$ is said to be self-complementary if $\mathcal{H} \cong \overline{\mathcal{H}}$, where $\overline{\mathcal{H}}$ is the complement of $\mathcal{H}$.

Construction of $\mathcal{H}$:
Replace each of the end vertices of P_4, the path on 4 vertices, by a copy of G and each of the internal vertices by a copy of $\overline{G}$. Join the vertices of these graphs by all possible edges whenever the corresponding vertices of P_4 are adjacent.

2. DISTANCE SPECTRUM OF $\mathcal{H}$

Theorem 1. *Let G be a connected k-regular graph on n vertices, with an adjacency matrix A and spectrum $\{k, \lambda_2, \ldots, \lambda_n\}$. Then the distance spectrum of $\mathcal{H}$ consists of $-(\lambda_i + 2)$ and $\lambda_i - 1$, $i = 2, 3, \ldots, n$, each with multiplicity 2, together with the numbers*

$$\frac{1}{2}\left[7n - 3 \pm \sqrt{(2k+1)^2 + 45n^2 - 12nk - 6n}\right]$$

and

$$-\frac{1}{2}\left[n + 3 \pm \sqrt{(2k+1)^2 + 5n^2 + 4nk + 2n}\right].$$

Proof. Let G be a connected k-regular graph on n vertices with an adjacency matrix A and spectrum $\{k, \lambda_2, \ldots, \lambda_n\}$. Let $\mathcal{H}$ be the self-complementary graph obtained from G by the above construction. Then the distance matrix D of $\mathcal{H}$ has the form

$$\begin{bmatrix} 2(J-I)-A & J & 2J & 3J \\ J & J-I+A & J & 2J \\ 2J & J & J-I+A & J \\ 3J & 2J & J & 2(J-I)-A \end{bmatrix}.$$

As a regular graph, G has the all-one vector j as an eigenvector corresponding to eigenvalue k, while all other eigenvectors are orthogonal to j. Also corresponding to the eigenvalue $\lambda \neq k$ of G, $\overline{G}$ has the eigenvalue $-1-\lambda$ such that both λ and $-1-\lambda$ have same multiplicities and eigenvectors.

Let λ be an arbitrary eigenvalue of the adjacency matrix of G with corresponding eigenvector x, such that $j^T x = 0$. Then $\begin{pmatrix} x & 0 & 0 & 0 \end{pmatrix}^T$ and $\begin{pmatrix} 0 & 0 & 0 & x \end{pmatrix}^T$ are the eigenvectors of D corresponding to eigenvalue $-\lambda-2$. Corresponding to an arbitrary eigenvalue λ of G, $-\lambda-2$ is an eigenvalue of D with multiplicity 2. Similarly $\begin{pmatrix} 0 & x & 0 & 0 \end{pmatrix}^T$ and $\begin{pmatrix} 0 & 0 & x & 0 \end{pmatrix}^T$ are the eigenvectors of D corresponding to the eigenvalue $\lambda - 1$.

In this way, forming eigenvectors of the form

$$\begin{pmatrix} x & 0 & 0 & 0 \end{pmatrix}^T, \begin{pmatrix} 0 & x & 0 & 0 \end{pmatrix}^T, \begin{pmatrix} 0 & 0 & x & 0 \end{pmatrix}^T, \begin{pmatrix} 0 & 0 & 0 & x \end{pmatrix}^T$$

we can construct a total of $4(n-1)$ mutually orthogonal eigenvectors of D. All these eigenvectors are orthogonal to the vectors

$$\begin{pmatrix} j & 0 & 0 & 0 \end{pmatrix}^T, \begin{pmatrix} 0 & j & 0 & 0 \end{pmatrix}^T, \begin{pmatrix} 0 & 0 & j & 0 \end{pmatrix}^T, \begin{pmatrix} 0 & 0 & 0 & j \end{pmatrix}^T.$$

The four remaining eigenvectors of D are of the form $\Psi = (\alpha j, \beta j, \gamma j, \delta j)^T$ for some $(\alpha, \beta, \gamma, \delta) \neq (0, 0, 0, 0)$.

Now, suppose that ν is an eigenvalue of D with an eigenvector Ψ. Then from $D\Psi = \nu\Psi$, we get

$$[2(n-1)-k]\,\alpha + n\beta + 2n\gamma + 3n\delta = \nu\alpha \tag{2}$$

$$n\alpha + (n-1+k)\,\beta + n\gamma + 2n\delta = \nu\beta \tag{3}$$

$$2n\alpha + n\beta + (n-1+k)\,\gamma + n\delta = \nu\gamma \tag{4}$$

$$3n\alpha + 2n\beta + n\gamma + [2(n-1)-k]\,\delta = \nu\delta\,. \tag{5}$$

Claim: $\alpha \neq 0$. If $\alpha = 0$, then by solving equations (3)–(5) we get $\beta = g_1\gamma$ and $\delta = g_2\gamma$ for some constants g_1 and g_2. Then using $\beta + 2\gamma + 3\delta = 0$, we obtain

$$\left[11n^2 + n\,(4k+2) + 12k^2 + 12k + 3\right]\gamma = 0$$

which implies that $\gamma = \beta = \delta = 0$, which is impossible.

Thus $\alpha \neq 0$ and without loss of generality we may set $\alpha = 1$.

Then by solving equations (3)–(5) for β, γ, and δ, and substituting these values into equation (2), we arrive at a biquadratic equation in ν:

$$\begin{aligned} & \left[\nu^2 - (7n-3)\,\nu + n\,(n+3k-9) - \left(k^2+k-2\right)\right] \\ \times \quad & \left[\nu^2 + (n+3)\,\nu - n\,(n+k-1) - \left(k^2+k-2\right)\right] = 0 \end{aligned}$$

whose solutions

$$\frac{1}{2}\left[7n - 3 \pm \sqrt{(2k+1)^2 + 45n^2 - 12nk - 6n}\right]$$

and

$$-\frac{1}{2}\left[n + 3 \pm \sqrt{(2k+1)^2 + 5n^2 + 4nk + 2n}\right]$$

as easily seen, represent the four remaining eigenvalues of D. Hence the theorem. $\square$

Corollary 1. *Let G be a connected k-regular graph on n vertices with an adjacency matrix A and spectrum $\{k, \lambda_2, \ldots, \lambda_n\}$. Let $\mathcal{H}$ be the self-complementary graph obtained from G by the above described construction. Then*

$$E_D(\mathcal{H}) = 7n - 3 + \sqrt{(2k+1)^2 + 5n^2 + 4nk + 2n} + \sum_{i=2}^{n} |\lambda_i + 2| + \sum_{i=2}^{n} |\lambda_i - 1| \ .$$

3. A PAIR OF D-EQUIENERGETIC SELF-COMPLEMENTARY GRAPHS

In this section we demonstrate the existence of a pair of D-equienergetic self-complementary graphs on n vertices for $n = 48t$ and $n = 24(2t+1)$ for all $t \geq 4$. For this we first prove:

Theorem 2. *For every $n \geq 8$, there exists a pair of 4-regular non-cospectral graphs on n vertices.*

Proof. We shall consider the following two cases.

Case 1: $n = 2t$, $t \geq 4$. In this case form two t-cycles $u_1u_2 \ldots u_t$ and $v_1v_2 \ldots v_t$ and join u_i to v_i for each i. Let $\mathcal{A}$ be the resulting graph. Let $\mathcal{B}_1$ be the graph obtained from $\mathcal{A}$ by making u_i adjacent with v_{i+1} for each i and $\mathcal{B}_2$ be obtained by making u_i adjacent with v_{i+2} for each i where suffix addition is modulo t. Then both $\mathcal{B}_1$ and $\mathcal{B}_2$ are 4-regular and the number of triangles in $\mathcal{B}_1$ is $2t$ and that in $\mathcal{B}_2$ is zero. Thus $\mathcal{B}_1$ and $\mathcal{B}_2$ are non-cospectral.

In Figure 1 we illustrate the above construction for $t = 4$.

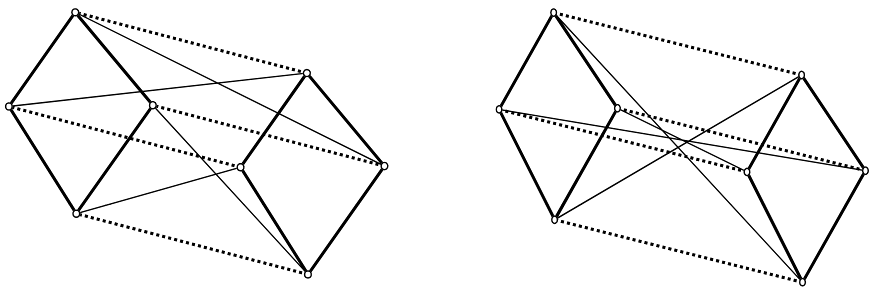

Figure 1. The graphs $\mathcal{B}_1$ and $\mathcal{B}_2$ in the case $t = 4$.

Case 2: $n = 2t + 1$, $t \geq 4$.

In this case form the $(t+1)$-cycle $v_1v_2 \ldots v_tv_{t+1}$ and the t-cycle $u_1u_2 \ldots u_t$. Now make v_{t-1} adjacent with v_1 and v_i with u_i, $i = 1, \ldots, t$. Then join v_j to u_{j+2}, $j = 2, \ldots, t-2$, v_t to u_2 and then v_{t+1} to u_1 and u_3. Let $\mathcal{F}_1$ be the resulting graph. Then $\mathcal{F}_1$ is 4-regular and contains two triangles $v_1v_2v_3$ and $v_5u_1v_1$ for $t = 4$ and only one triangle $v_{t+1}u_1v_1$ for $t \geq 5$.

To get the other 4-regular graph, form the $(2t+1)$-cycle $v_1v_2 \ldots v_tv_{t+1} \ldots v_{2t+1}$. Join v_i to v_{i+2} , $i = 1, 3, 5, \ldots, 2t+1, 2, 4, 6, \ldots, 2t$. Let $\mathcal{F}_2$ be the resulting graph. Then it is 4-regular and contains $2t+1$ triangles. Thus the graphs $\mathcal{F}_1$ and $\mathcal{F}_2$ are not cospectral. $\square$

In Figure 2 we illustrate the above construction for $t = 4$.

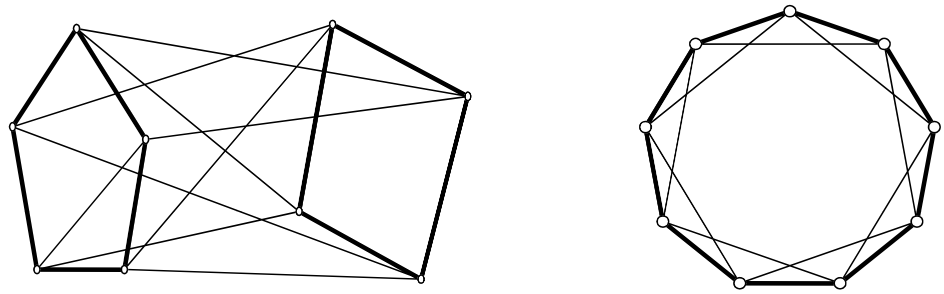

Figure 2. The graphs $\mathcal{F}_1$ and $\mathcal{F}_2$ in the case $t = 4$.

Theorem 3. *Let G be a connected 4-regular graph on n vertices, with an adjacency matrix A and spectrum $\{4, \lambda_2, \ldots, \lambda_n\}$. Let $H = L^2(G)$ and $\mathcal{H}$ be the P_4 self-complementary graph obtained from H, according to the above described construction. Then*

$$E_D(\mathcal{H}) = 3[8(3n - 1) + \sqrt{20n^2 + 28n + 49}] \ .$$

Proof follows from Theorem 1, Lemma 1, and the fact that both $\lambda_i + 3r - 4$ and $\lambda_i + 3r - 7$ are positive when $r = 4$. $\square$

Theorem 4. *For every $n = 48t$ and $n = 24(2t + 1)$, $t \geq 4$, there exists a pair of D-equienergetic self-complementary graph.*

Proof. Case 1: $n = 48t$

Let $\mathcal{B}_1$ and $\mathcal{B}_2$ be the two non-cospectral 4-regular graphs on $2t$ vertices as given by Theorem 2. Let $\mathbb{B}_1$ and $\mathbb{B}_2$ respectively denote their second iterated line graphs. Then both are on $12t$ vertices and are 6-regular. Let $\mathfrak{B}_1$ and $\mathfrak{B}_2$ be the respective self-complementary graphs on $48t$ vertices. Then by Theorem 3, $\mathfrak{B}_1$ and $\mathfrak{B}_2$ are D-equienergetic.

The other case $n = 24(2t + 1)$ can be proven in a similar manner by considering the two non-cospectral 4-regular graphs on $2t+1$ vertices whose structure is outlined in Theorem 2. $\square$

4. D-ENERGY OF SOME SELF-COMPLEMENTARY GRAPHS

The D-energy of some self-complementary graphs $\mathcal{H}$ is easily deduced from the adjacency spectra of the respective parent graphs G.

1. If $G \cong K_n$, the complete graph on n vertices, then

$$E_D(\mathcal{H}) = \begin{cases} 4 + 2\sqrt{10} & \text{for } n = 1 \\ 6 + 3\sqrt{17} + \sqrt{41} & \text{for } n = 2 \\ 22 + 2\sqrt{85} & \text{for } n = 3 \\ 13n - 9 + \sqrt{13n^2 - 6n + 1} & \text{for } n \geq 4 . \end{cases}$$

2. If $G \cong K_{p,p}$, the complete bipartite graph on $n = 2p$ vertices, then

$$E_D(\mathcal{H}) = 15n - 17 + \sqrt{8n^2 + 4n + 1} .$$

3. If $G \cong CP(n)$, the cocktail party graph on n vertices, then

$$E_D(\mathcal{H}) = 13n - 9 + \sqrt{13n^2 - 18n + 9} .$$

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