

Triply Equienergetic Graphs

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Abstract

Pairs of non-cospectral graphs are constructed, having equal energy (E), Laplacian energy (LE), and distance energy (DE). These seem to be the first examples of “triply equienergetic graphs”. We construct a family of integral circulant graphs (ICG) of order $n = 2pq$, where $p > q > 2$ are prime numbers, $G_n = ICG(n, \{1, 2\})$ and $H_n = ICG(n, \{p, 2p, q, 2q\})$, for which $E(G_n) = E(H_n) = 8(p-1)(q-1)$, $LE(G_n) = LE(H_n) = 8(p-1)(q-1)$, and $DE(G_n) = DE(H_n) = 8(p-1)(q-1) + 4pq$.

1 Introduction

Let \mathbf{A} be the adjacency matrix of a simple graph G , and let $\lambda_1, \lambda_2, \dots, \lambda_n$ be its eigenvalues. These are said to be the eigenvalues of the graph G and form its spectrum [12]. The energy $E(G)$ of the graph G is defined as the sum of the absolute values of its eigenvalues [16],

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

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The concept of graph energy originates from the Hückel molecular orbital approximation for the total π -electron energy (for details see [17]). In the last 5–10 years research on graph energy became a popular theme in both mathematics and mathematical chemistry (see the recent surveys [18, 19], the papers published in this issue of *MATCH*, and the references cited therein).

Motivated by the successes of the theory of graph energy, energy-like quantities, based on the eigenvalues of graph matrices other than the adjacency matrix, have been proposed. Of these we are concerned here with the *Laplacian graph energy* (LE) and the *distance energy* (DE).

Let \mathbf{L} be the Laplacian matrix of the graph G , and $\mu_1, \mu_2, \dots, \mu_n$ be its eigenvalues [14, 15, 33]. Then the Laplacian energy of G is [1, 20, 52, 53]

$$LE = LE(G) = \sum_{i=1}^n \left| \mu_i - \frac{2m}{n} \right|$$

where n and m denote the number of vertices and edges. For some recent research on LE see [13, 40, 45, 49].

The distance matrix \mathbf{D} of a graph G is the square matrix whose (i, j) -entry is the distance between the i -th and j -th vertex of G . The eigenvalues $\rho_1, \rho_2, \dots, \rho_n$ of the distance matrix are said to be the distance or D -eigenvalues of the underlying graph and form its distance spectrum. The *distance energy* of a graph G is the sum of absolute values of the D -eigenvalues [26],

$$DE = DE(G) = \sum_{i=1}^n |\rho_i|.$$

For some recent research on DE see [9, 23, 24, 34, 35, 46, 51]. The distance energy was shown to be a useful molecular structure-descriptor in QSPR modeling [11].

Two graphs G_1 and G_2 are said to be cospectral if their spectra coincide [12]. In full analogy we speak of pairs of Laplacian cospectral and distance cospectral graphs. Evidently, cospectral graphs have equal energies, Laplacian cospectral graphs have equal Laplacian energies, and distance cospectral graphs have equal distance energies. However, there exist pairs of non-cospectral graphs with equal energy. These will be referred to as **A**-equienergetic [2, 10]. Analogously, there exist pairs of graphs with equal Laplacian energy, so-called **L**-equienergetic graphs, and with equal distance energy, so-called **D**-equienergetic graphs.

In what follows we are interested only in non-cospectral equienergetic graphs, and non-cospectrality is tacitly assumed.

Many recent papers are devoted to finding and constructing of **A**-equienergetic graphs, e. g., [8, 27, 28, 30, 32, 36, 37, 38, 44, 50]. In [45] **L**-equienergetic graphs are obtained, whereas the papers [25, 31, 35] report on **D**-equienergetic graphs.

Using a computer search on graphs with < 10 vertices, we concluded that there are no pairs of **A**-, **L**-, and **D**-equienergetic graphs.

One of the fundamental properties of Laplacian energy is that in the case of regular graphs LE is equal to E [20]. Therefore, if two regular graphs G_1 and G_2 are **A**-equienergetic, then these automatically are also **L**-equienergetic. A systematic method for constructing families of **A**-equienergetic regular graphs was elaborated in [37, 38]: If G_a and G_b are any two regular graphs of the same order and of the same degree, then their second line graphs (i. e., the line graph of the line graph) are both **A**- and **L**-equienergetic.

Until now, to our best knowledge, no pairs of graphs were found that are both **A**-equienergetic, **L**-equienergetic, and **D**-equienergetic. We now construct such triply equienergetic graphs.

In this note, we present a family of pairs (G_n, H_n) for $n = 2pq$, with $p > q > 2$ being prime numbers, such that G_n and H_n are **A**-equienergetic, **D**-equienergetic, and **L**-equienergetic. Based on this construction, one can establish similar pairs of integral circulant graphs, and use line graphs or graph products for constructing further pairs of equienergetic graphs. These examples of integral circulant graphs represent a fruitful connection between Mathematical chemistry, Graph theory, and Number theory.

2 Preliminaries

A graph is said to be *circulant* if its adjacency matrix is circulant [7, 42, 47]. A graph is called *integral* if all eigenvalues of its adjacency matrix are integers. Integral graphs were extensively studied in the literature and there was a vast research for specific classes of graphs with integral spectrum [3].

Integral circulant graphs were imposed as potential candidates for modeling quan-

tum spin networks with periodic dynamics. For the certain quantum spin system, the necessary condition for the existence of perfect state transfer in qubit networks is the periodicity of the system dynamics (see [41]). Various properties of integral circulant graphs were investigated in [4, 5, 6, 29, 43].

Integral circulant graphs are the natural extension of the class of unitary Cayley graphs. Let D be a set of positive, proper divisors of the integer $n > 1$. Define the graph $ICG(n, D)$ so that its vertex set be $Z_n = \{0, 1, \dots, n-1\}$ and its edge set

$$\{\{a, b\} \mid a, b \in Z_n, \gcd(a-b, n) \in D\}.$$

The graph $ICG(n, D)$ is regular of degree $\sum_{d \in D} \varphi(n/d)$, where $\varphi(n)$ denotes the Euler function. These graphs are highly symmetric and have some remarkable properties connecting graph theory and number theory.

Let ω denote a complex primitive n -th root of unity. It is proven in [29] that the eigenvalues of $ICG(n, D)$ are integral and are given by

$$\lambda_i = \sum_{d \in D} c(i, n/d) \quad (1)$$

where

$$c(i, n) = \sum_{1 \leq j < n, \gcd(j, n)=1} \omega^{ij}, \quad 0 \leq i \leq n-1.$$

The arithmetic function $c(i, n)$ is a Ramanujan sum, and for integers i and n these sums have only integral values,

$$c(i, n) = \varphi(n) \cdot \frac{\mu(t_i)}{\varphi(t_i)} \quad \text{and} \quad t_i = \frac{n}{\gcd(i, n)}$$

where μ denotes the Möbius function,

$$\mu(n) = \begin{cases} (-1)^k & \text{if } n \text{ is a square-free positive integer} \\ 0 & \text{if } n \text{ is not square-free} \end{cases}.$$

In [22] and [39] the authors analyze the energy of integral circulant graphs, and establish conditions for $ICG(n, D)$ to be hyperenergetic. (Recall that an n -vertex graph is said to be hyperenergetic if its energy is greater than $2n-2$ [21, 47, 48]).

The distance spectrum of $ICG(n, D)$ is given by [23]:

$$\rho_i = 1 \cdot \sum_{j=1}^{s_1} c\left(r, \frac{n}{d_j^{(1)}}\right) + 2 \cdot \sum_{j=1}^{s_2} c\left(r, \frac{n}{d_j^{(2)}}\right) + \dots + \text{diam}(G) \cdot \sum_{j=1}^{s_{\text{diam}(G)}} c\left(r, \frac{n}{d_j^{(\text{diam}(G))}}\right) \quad (2)$$

where

$$D^{(p)} = \{d_1^{(p)}, d_2^{(p)}, \dots, d_{s_p}^{(p)}\}, \quad 1 \leq p \leq \text{diam}(G)$$

is the set of divisors determined by the vertices on distance p from the starting vertex 0.

3 Main result

Let $n = 2pq$, where $p > q > 2$ are arbitrary prime numbers. Consider the following integral circulant graphs

$$G_n = ICG(2pq, \{1, 2\}) \quad \text{and} \quad H_n = ICG(2pq, \{p, 2p, q, 2q\}) .$$

Based on the formula (1), the adjacency eigenvalues of G_n and H_n are

$$\lambda_i^G = c(i, 2pq) + c(i, pq), \quad i = 1, 2, \dots, n .$$

and

$$\lambda_i^H = c(i, p) + c(i, 2p) + c(i, q) + c(i, 2q), \quad i = 1, 2, \dots, n .$$

For the index i , we have eight possibilities for the greatest common divisor of i and $2pq$. Therefore, the adjacency spectrum of G_n is

$$\lambda_i^G = \begin{cases} 0 & \text{if } \gcd(i, 2pq) = 1 \\ 2 & \text{if } \gcd(i, 2pq) = 2 \\ 0 & \text{if } \gcd(i, 2pq) = p \\ 0 & \text{if } \gcd(i, 2pq) = q \\ -2(p-1) & \text{if } \gcd(i, 2pq) = 2p \\ -2(q-1) & \text{if } \gcd(i, 2pq) = 2q \\ 0 & \text{if } \gcd(i, 2pq) = pq \\ 2(p-1)(q-1) & \text{if } \gcd(i, 2pq) = 2pq \end{cases}$$

Analogously, the adjacency spectrum of H_n is

$$\lambda_i^H = \begin{cases} 0 & \text{if } \gcd(i, 2pq) = 1 \\ -4 & \text{if } \gcd(i, 2pq) = 2 \\ 0 & \text{if } \gcd(i, 2pq) = p \\ 0 & \text{if } \gcd(i, 2pq) = q \\ 2(p-2) & \text{if } \gcd(i, 2pq) = 2p \\ 2(q-2) & \text{if } \gcd(i, 2pq) = 2q \\ 0 & \text{if } \gcd(i, 2pq) = pq \\ 2(p+q-2) & \text{if } \gcd(i, 2pq) = 2pq \end{cases}$$

The energy of G_n is thus

$$\begin{aligned} E(G_n) &= (p-1)(q-1) \cdot 0 + (p-1)(q-1) \cdot 2 + (q-1) \cdot 0 + (p-1) \cdot 0 \\ &\quad + (q-1) \cdot (2(p-1)) + (p-1) \cdot (2(q-1)) + 1 \cdot 0 + 1 \cdot (2(p-1)(q-1)) \\ &= 8(p-1)(q-1) . \end{aligned}$$

The energy of H_n is

$$\begin{aligned} E(H_n) &= (p-1)(q-1) \cdot 0 + (p-1)(q-1) \cdot 4 + (q-1) \cdot 0 + (p-1) \cdot 0 \\ &\quad + (q-1) \cdot (2(p-2)) + (p-1) \cdot (2(q-2)) + 1 \cdot 0 + 1 \cdot (2(p+q-2)) \\ &= 8(p-1)(q-1) . \end{aligned}$$

We see that G_n and H_n are non-cospectral graphs with equal energy. Because G_n and H_n are regular, it follows that $E(G_n) = LE(G_n)$ and $E(H_n) = LE(H_n)$. Thus, G_n and H_n are both **A**-equienergetic and **L**-equienergetic.

The graphs G_n and H_n are generated from divisor subsets $\{1, 2\}$ and $\{p, 2p, q, 2q\}$, so it follows that the diameter of both graphs is two.

Based on the formula (2), the distance eigenvalues of G_n and H_n are

$$\rho_i^G = c(i, 2pq) + c(i, pq) + 2[c(i, p) + c(i, 2p) + c(i, q) + c(i, 2q) + c(i, 2)] , \quad i = 1, 2, \dots, n .$$

and

$$\rho_i^H = c(i, p) + c(i, 2p) + c(i, q) + c(i, 2q) + 2[c(i, 2pq) + c(i, pq) + c(i, 2)] , \quad i = 1, 2, \dots, n .$$

For the index i , we have eight possibilities for the greatest common divisor of i and $2pq$. Therefore, the distance spectrum of G_n is

$$\rho_i^G = \begin{cases} -2 & \text{if } \gcd(i, 2pq) = 1 \\ -4 & \text{if } \gcd(i, 2pq) = 2 \\ -2 & \text{if } \gcd(i, 2pq) = p \\ -2 & \text{if } \gcd(i, 2pq) = q \\ 2(p-2) & \text{if } \gcd(i, 2pq) = 2p \\ 2(q-2) & \text{if } \gcd(i, 2pq) = 2q \\ -2 & \text{if } \gcd(i, 2pq) = pq \\ 2(p-1)(q-1) + 4(p+q-2) + 2 & \text{if } \gcd(i, 2pq) = 2pq \end{cases}$$

Analogously, the distance spectrum of H_n is

$$\rho_i^H = \begin{cases} -2 & \text{if } \gcd(i, 2pq) = 1 \\ 4 & \text{if } \gcd(i, 2pq) = 2 \\ -2 & \text{if } \gcd(i, 2pq) = p \\ -2 & \text{if } \gcd(i, 2pq) = q \\ -2(p-1) & \text{if } \gcd(i, 2pq) = 2p \\ -2(q-1) & \text{if } \gcd(i, 2pq) = 2q \\ -2 & \text{if } \gcd(i, 2pq) = pq \\ 4(p-1)(q-1) + 2(p+q-2) + 2 & \text{if } \gcd(i, 2pq) = 2pq \end{cases}$$

The D -energies of G_n and H_n are

$$\begin{aligned} DE(G_n) &= (p-1)(q-1) \cdot 2 + (p-1)(q-1) \cdot 4 + (q-1) \cdot 2 + (p-1) \cdot 2 \\ &+ (q-1) \cdot (2(p-2)) + (p-1) \cdot (2(q-2)) + 1 \cdot 2 \\ &+ 1 \cdot (2(p-1)(q-1) + 4(p+q-2) + 2) \\ &= 4(3pq - 2p - 2q + 2) = E(G_n) + 2n \end{aligned}$$

and

$$\begin{aligned} DE(H_n) &= (p-1)(q-1) \cdot 2 + (p-1)(q-1) \cdot 4 + (q-1) \cdot 2 + (p-1) \cdot 2 \\ &+ (q-1) \cdot (2(p-1)) + (p-1) \cdot (2(q-1)) + 1 \cdot 2 \\ &+ 1 \cdot (4(p-1)(q-1) + 2(p+q-2) + 2) \\ &= 4(3pq - 2p - 2q + 2) = E(H_n) + 2n . \end{aligned}$$

Thus, we see that the graphs G_n and H_n are non-cospectral and **D**-equienergetic.

In Figure 1 is depicted the smallest pair of such triply equienergetic graphs, possessing 30 vertices.

Similarly, one can prove that the integral circulant graphs $ICG(8p, \{1, 2\})$ and $ICG(8p, \{4, 8, p, 2p\})$ are **A**-, **L**-, and **D**-equienergetic.

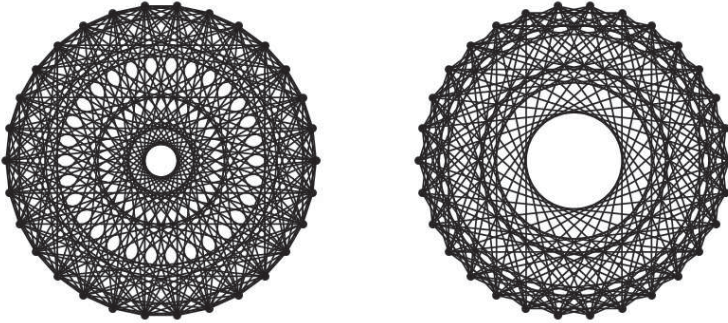


Figure 1: A pair of triply equienergetic integral circulant graphs on 30 vertices.

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