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ISI-Equienergetic Graphs

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Abstract: The ISI-energy $\varepsilon_{isi}(G)$ of a graph $G = (V, E)$ is the sum of the absolute values of the eigenvalues of the ISI-matrix $\mathcal{C}(G) = [c_{ij}]_{n\times n}$ in which $c_{ij} = \frac{d(v_i)d(v_j)}{d(v_i)+d(v_j)}$ if $v_iv_j \in E(G)$ and $c_{ij} = 0$ otherwise. $d(v_i)$ denotes the degree of vertex $v_i \in V$. As a class of graph energy, ISI-energy can be utilized to ascertain the general energy of conjugated carbon molecules. Two non-isomorphic graphs of the same order are said to be ISI-equienergetic if their ISI-energies are equal. In this paper, we construct pairs of connected, ISI-noncospectral, ISI-equienergetic graphs of order n for all $n \geq 9$. In addition, for n-vertex $r(r \geq 3)$-regular graph G, and for each $k \geq 2$, we obtain $\varepsilon_{isi}(\overline{L^k(G)})$, depending only on n and r. This result enables a systematic construction of pairs of ISI-noncospectral graphs of the same order, having equal ISI-energies.

Keywords: ISI-matrix; energy; ISI-energy; ISI-equienergetic; ISI-noncospectral

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1. Introduction

A graph $G = (V(G), E(G))$ is a mathematical structure composed of two finite sets $V(G)$ and $E(G)$. The elements of $V(G)$ are called *vertices* (or *nodes*), and the elements of $E(G)$ are called *edges*. For $v_i \in V(G)$, $N(v_i)$ denotes the set of its neighbors in G, and the degree of v_i is $d(v_i) = |N(v_i)|$. An *n-vertex graph* denotes the graph of order n. A graph with only r-vertices is called an *r-regular* graph. Throughout the article, only finite simple undirected graphs are considered. We use Bondy and Murty [1] for terminology and notations not defined here.

The *ISI index* is an interesting topological index which can distinctively forecast the superficial area for isomers of octanes [2]. The ISI index of graph G is defined as

$$ISI(G) = \sum_{v_iv_j \in E(G)} \frac{d(v_i)d(v_j)}{d(v_i) + d(v_j)}.$$

The *ISI-matrix* $\mathbf{C} = \mathbf{C}(G)$ of the graph G is defined as the matrix with entries [3–5]:

$$c_{ij} := \begin{cases} \frac{d(v_i)d(v_j)}{d(v_i)+d(v_j)}, & if\ v_iv_j \in E(G) \\ 0, & otherwise. \end{cases}$$

Note that $\mathbf{C}$ is a modification of the classical adjacency matrix.

The characteristic polynomial of $\mathbf{C}(G)$ is called the *ISI-characteristic polynomial* of n-vertex graph G, defined as $\Phi(\mathbf{C}(G), \mu) = det(\mu\mathbf{I}_n - \mathbf{C}(G))$, where $\mathbf{I}_n$ is the unit matrix of order n. The eigenvalues of the ISI-matrix $\mathbf{C}(G)$, denoted by $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n$, are said to be the *ISI-eigenvalues* of G. In [3], we proved that the sum of the ISI-eigenvalues of G is zero.

Let **A** denote the adjacency matrix of a graph G of order n. Because **A** and **C** are real symmetric matrices, their eigenvalues are real numbers. Denote by $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ the ordered eigenvalues of **A**. The characteristic polynomial of the matrix **A** is the *characteristic polynomial* of G, denoted by $\Phi(G, \lambda) = det(\lambda I - \mathbf{A})$. If $\lambda_1, \lambda_2, \ldots, \lambda_k$ are the distinct eigenvalues of G with respective multiplicities $m_1, m_2, \ldots, m_k$, then the spectrum of G is denoted by

$$Spec(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \ldots & \lambda_k \\ m_1 & m_2 & \ldots & m_k \end{pmatrix}.$$

Topological molecular descriptors based on eigenvalues are widely used in chemical research [6,7]. It is possible that the graph energy [8–10] is the most studied descriptor of this kind, which is mainly used to describe the stability of conjugated molecules. The *energy* [8] of an n-vertex graph G is defined as

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

Generalizing the energy concept to the ISI-matrix, the *ISI-energy* [4,11] is defined as below

$$\varepsilon_{isi} = \varepsilon_{isi}(G) = \sum_{i=1}^{n} |\mu_i| \,. \tag{2}$$

It is worth noting that $\varepsilon(G)$ and $\varepsilon_{isi}(G)$ of graphs are closely linked, and we can determine $\varepsilon(G)$ by means of $\varepsilon_{isi}(G)$. Consequently, the $\varepsilon_{isi}(G)$ study is not only of theoretical meaning but also of realistic value.

When two graphs G_1 and G_2 have different structures, it is taken for granted that $\varepsilon_{isi}(G_1) \neq \varepsilon_{isi}(G_2)$. Nevertheless, it is not always true by observation. That is, two structurally different graphs can have equal ISI-energy. For example, take into account the cycles C_3 and C_4. The ISI-eigenvalues of C_3 and C_4 are $1, -\frac{1}{2}, \frac{1}{2}$ and $1, 0, 0, 1$, respectively. Hence, $\varepsilon_{isi}(C_3) = \varepsilon_{isi}(C_4)$. This observation results in the conception of ISI-equienergetic graphs.

Two non-isomorphic graphs are said to be *ISI-cospectral* if they have the same ISI-eigenvalues. The graphs G_1 and G_2 are said to be *ISI-equienergetic* if $\varepsilon_{isi}(G_1) = \varepsilon_{isi}(G_2)$. Apparently, two ISI-cospectral graphs must be ISI-equienergetic, but the converse is not always true in common cases. Thus, we are interested in the construction of ISI-equienergetic pairs of graphs which are ISI-noncospectral.

If we do not restrict two graphs to have the same number of vertices, it is extremely simple to construct ISI-noncospectral, ISI-equienergetic graphs. Let G be any graph with ISI-spectrum $\mu_1, \mu_2, \ldots, \mu_n$, and let G_0 be the graph obtained by adding arbitrarily $t (t \geq 1)$ number of isolated vertices to G, then the spectrum of G_0 consists of the numbers $\mu_1, \mu_2, \ldots, \mu_n, \mu_{n+1} = 0, \mu_{n+2} = 0, \ldots, \mu_{n+t} = 0$. Thus, G and G_0 are not ISI-cospectral but $\varepsilon_{isi}(G) = \varepsilon_{isi}(G_0)$.

If we also require this kind of graph to have the same order and equal number of edges (which is of great value in chemical applications), the problem becomes not so easy. As we know, up to now, there exists no systematic approach for constructing pairs (or larger families) of ISI-equienergetic graphs. Therefore, it is interesting to obtain ISI-noncospectral graphs on the same number of vertices having equal ISI-energy. Our results can quickly obtain the ISI-energy of the ISI-noncospectral, ISI-equienergetic graphs, which can greatly reduce the workload of calculating the ISI-energy of graphs.

This paper is organized as follows. We first obtain the characteristic polynomial of the ISI-matrix of the join of two regular graphs and thereby construct pairs of ISI-noncospectral, ISI-equienergetic graphs on n vertices for all $n \geq 9$. Furthermore, for n-vertex $r(r \geq 3)$-regular graph G, and for each $k \geq 2$, we obtain $\varepsilon_{isi}(\overline{L^k(G)})$, depending only on n and r. This result enables a systematic construction of pairs of ISI-noncospectral graphs of the same order, having equal ISI-energies.

2. ISI-Equienergetic Graphs

In this section, we pay our attention to constructions of ISI-noncospectral, ISI-equienergetic graphs.

Let G and H be two graphs. The join $G+H$ of G and H is the graph with vertex set $V(G+H) = V(G) \cup V(H)$, and the edge set $E(G+H)$ is obtained by joining each of the vertices of $V(G)$ to all the vertices of $V(H)$.

We denote by $\mathbf{J}_{n_1 \times n_2}$ the $n_1 \times n_2$ matrix having all its entries as 1. It can be noted that if G is a k-regular graph, then $\mathbf{C}(G) = \frac{k}{2}\mathbf{A}(G)$.

In the following theorem, we give the ISI-characteristic polynomial of $G+H$ when both G and H are regular graphs.

Theorem 1. *Let G_i be an n_i-vertex r_i-regular graph for $i = 1, 2$. Then, the ISI-characteristic polynomial of $G = G_1 + G_2$ is*

$$\Phi(\mathbf{C}(G), \mu) = \frac{(\mu - X)(\mu - Y) - n_1 n_2 a^2}{(\mu - X)(\mu - Y)} \Phi(\mathbf{C}'(G_1), \mu)\Phi(\mathbf{C}'(G_2), \mu), \tag{3}$$

where $X = \frac{(r_1+n_2)r_1}{2}$, $Y = \frac{(r_2+n_1)r_2}{2}$, $a = \frac{(n_1+r_2)(n_2+r_1)}{n_1+n_2+r_2+r_1}$, $\mathbf{C}'(G_1) = \frac{r_1+n_2}{r_1}\mathbf{C}(G_1)$, $\mathbf{C}'(G_2) = \frac{r_2+n_1}{r_2}\mathbf{C}(G_2)$.

Proof. As G_i is an n_i-vertex r_i-regular graph for $i = 1, 2$, we have

$$\mathbf{C}(G_1 + G_2) = \begin{pmatrix} \mathbf{C}'(G_1) & a\mathbf{J}_{n_1 \times n_2} \\ a\mathbf{J}_{n_2 \times n_1} & \mathbf{C}'(G_2) \end{pmatrix}, \tag{4}$$

where $a = \frac{(n_1+r_2)(n_2+r_1)}{n_1+n_2+r_2+r_1}$.

And we obtain

$$\Phi(\mathbf{C}(G), \mu) = det(\mu\mathbf{I}_n - \mathbf{C}(G)) = \begin{vmatrix} \mu\mathbf{I}_{n_1} - \mathbf{C}'(G_1) & -a\mathbf{J}_{n_1 \times n_2} \\ -a\mathbf{J}_{n_2 \times n_1} & \mu\mathbf{I}_{n_2} - \mathbf{C}'(G_2) \end{vmatrix}. \tag{5}$$

Let

$$c_{ij} := \begin{cases} \frac{d(v_i)d(v_j)}{d(v_i)+d(v_j)}, & if\ v_iv_j \in E(G_1) \\ 0, & otherwise. \end{cases}$$

and

$$c'_{ij} := \begin{cases} \frac{d(u_i)d(u_j)}{d(u_i)+d(u_j)}, & if\ u_iu_j \in E(G_2) \\ 0, & otherwise. \end{cases}$$

Determinant (5) can be written as

$$\begin{vmatrix} \mu & -c_{12} & \dots & -c_{1n_1} & -a & -a & \dots & -a \\ -c_{21} & \mu & \dots & -c_{1n_1} & -a & -a & \dots & -a \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -c_{n_11} & -c_{n_12} & \dots & \mu & -a & -a & \dots & -a \\ -a & -a & \dots & -a & \mu & -c'_{12} & \dots & -c'_{1n_2} \\ -a & -a & \dots & -a & -c'_{21} & \mu & \dots & -c'_{2n_2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -a & -a & \dots & -a & -c'_{n_21} & -c'_{n_22} & \dots & \mu \end{vmatrix} \tag{6}$$

It is obvious that

$$\sum_{j=1}^{n_1} c_{ij} = \frac{(r_1 + n_2)r_1}{2} = X \tag{7}$$

for $i = 1, 2, \ldots, n_1$, and

$$\sum_{j=1}^{n_2} c'_{ij} = \frac{(r_2 + n_1)r_2}{2} = Y \tag{8}$$

for $i = 1, 2, \ldots, n_2$.

By subtracting the row (n_1+1) from the rows $(n_1+2), (n_1+3), \ldots, (n_1+n_2)$ of determinant (6), we obtain determinant (9).

$$\begin{vmatrix} \mu & -c_{12} & \ldots & -c_{1n_1} & -a & -a & \ldots & -a \\ -c_{21} & \mu & \ldots & -c_{1n_1} & -a & -a & \ldots & -a \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -c_{n_11} & -c_{n_12} & \ldots & \mu & -a & -a & \ldots & -a \\ -a & -a & \ldots & -a & \mu & -c'_{12} & \ldots & -c'_{1n_2} \\ 0 & 0 & \ldots & 0 & -\mu - c'_{21} & \mu + c'_{12} & \ldots & -c'_{2n_2} + c'_{1n_2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 & -\mu - c'_{n_21} & -c'_{n_22} + c'_{12} & \ldots & \mu + c'_{1n_2} \end{vmatrix} \tag{9}$$

Add the columns $(n_1+2), (n_1+3), \ldots, (n_1+n_2)$ to the column (n_1+1) of determinant (9), we obtain determinant (10).

$$\begin{vmatrix} \mu & -c_{12} & \ldots & -c_{1n_1} & -an & -a & \ldots & -a \\ -c_{21} & \mu & \ldots & -c_{1n_1} & -an & -a & \ldots & -a \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -c_{n_11} & -c_{n_12} & \ldots & \mu & -an & -a & \ldots & -a \\ -a & -a & \ldots & -a & \mu - Y & -c'_{12} & \ldots & -c'_{1n_2} \\ 0 & 0 & \ldots & 0 & 0 & \mu + c'_{12} & \ldots & -c'_{2n_2} + c'_{1n_2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 & 0 & -c'_{n_22} + c'_{12} & \ldots & \mu + c'_{1n_2} \end{vmatrix} \tag{10}$$

For convenience, we let

$$|\mathbf{B}| = \begin{vmatrix} \mu + c'_{12} & -c'_{23} + c'_{13} & \ldots & -c'_{2n_2} + c'_{1n_2} \\ -c'_{32} + c'_{12} & \mu + c'_{13} & \ldots & -c'_{3n_2} + c'_{1n_2} \\ \vdots & \vdots & \vdots & \vdots \\ -c'_{n_22} + c'_{12} & -c'_{n_23} + c'_{13} & \ldots & \mu + c'_{1n_2} \end{vmatrix} \tag{11}$$

Subtract the first row from the rows $2, 3, \ldots, n_1$ of determinant (10), and we obtain determinant (12).

$$\begin{vmatrix} \mu & -c_{12} & \ldots & -c_{1n_1} & -an & -a & \ldots & -a \\ -c_{21} - \mu & \mu + c_{12} & \ldots & 0 & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -c_{n_11} - \mu & -c_{n_12} + c_{12} & \ldots & \mu + c_{1n_1} & 0 & 0 & \ldots & 0 \\ -a & -a & \ldots & -a & \mu - Y & -c'_{12} & \ldots & -c'_{1n_2} \\ 0 & 0 & \ldots & 0 & 0 & \mu + c'_{12} & \ldots & -c'_{2n_2} + c'_{1n_2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 & 0 & -c'_{n_22} + c'_{12} & \ldots & \mu + c'_{1n_2} \end{vmatrix} \tag{12}$$

Add the columns $2, 3, \ldots, n_1$ to the first column of determinant (12), and we arrive at determinant (13).

$$\begin{vmatrix} \mu - X & -c_{12} & \dots & -c_{1n_1} & -an_2 \\ 0 & \mu + c_{12} & \dots & -c_{1n_1} + c_{1n_1} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & -c_{n_1 2} + c_{12} & \dots & \mu + c_{1n_1} & 0 \\ -an_1 & -a & \dots & -a & \mu - Y \end{vmatrix} |\mathbf{B}| \tag{13}$$

Expand determinant (13) along the first column to obtain (14):

$$det(\mu \mathbf{I}_n - \mathbf{C}(G)) = (\mu - X)|\mathbf{D}_1| - (-1)^{n_1} an_1 |\mathbf{D}_2|)|\mathbf{B}| \tag{14}$$

where

$$|\mathbf{D}_1| = \begin{vmatrix} \mu + c_{12} & -c_{23} + c_{13} & \dots & -c_{1n_1} + c_{1n_1} & 0 \\ -c_{32} + c_{12} & \mu + c_{13} & \dots & -c_{3n_1} + c_{1n_1} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -c_{n_1 2} + c_{12} & -c_{n_1 3} + c_{13} & \dots & \mu + c_{1n_1} & 0 \\ -a & -a & \dots & -a & \mu - Y \end{vmatrix}$$

$$|\mathbf{D}_2| = \begin{vmatrix} -c_{12} & -c_{13} & \dots & -c_{1n_1} & -an_2 \\ \mu + c_{12} & -c_{23} + c_{13} & \dots & -c_{2n_1} + c_{1n_1} & 0 \\ -c_{32} + c_{12} & \mu + c_{13} & \dots & -c_{3n_1} + c_{1n_1} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -c_{n_1 2} + c_{12} & -c_{n_1 3} + c_{13} & \dots & \mu + c_{1n_1} & 0 \end{vmatrix}$$

Let

$$|\mathbf{A}| = \begin{vmatrix} \mu + c_{12} & -c_{23} + c_{13} & \dots & -c_{2n_1} + c_{1n_1} \\ -c_{32} + c_{12} & \mu + c_{13} & \dots & -c_{3n_1} + c_{1n_1} \\ \vdots & \vdots & \vdots & \\ -c_{n_1 2} + c_{12} & -c_{n_1 3} + c_{13} & \dots & \mu + c_{1n_1} \end{vmatrix}$$

Expression (14) can be written as

$$\begin{aligned} det(\mu \mathbf{I}_n - \mathbf{C}(G)) &= ((\mu - X)(\mu - Y)|\mathbf{A}| - (-1)^{n_1} an_1 (-1)^{n_1+1}(-n_2 a)|\mathbf{A}|)|\mathbf{B}| \\ &= ((\mu - X)(\mu - Y) - n_1 n_2 a^2))|\mathbf{A}||\mathbf{B}| \end{aligned} \tag{15}$$

On the other hand, the determinant $|\mathbf{A}|$ can be written as

$$|\mathbf{A}| = \frac{1}{\mu - X} \begin{vmatrix} \mu - X & -c_{12} & -c_{13} & \dots & -c_{1n_1} \\ 0 & \mu + c_{12} & -c_{23} + c_{13} & \dots & -c_{2n_1} + c_{1n_1} \\ 0 & -c_{32} + c_{12} & \mu + c_{13} & \dots & -c_{3n_1} + c_{1n_1} \\ \vdots & \vdots & \vdots & \vdots & \\ 0 & -c_{n_1 2} + c_{12} & -c_{n_1 3} + c_{13} & \dots & \mu + c_{1n_1} \end{vmatrix}$$

Let

$$|\mathbf{H}| = \begin{vmatrix} \mu - X & -c_{12} & -c_{13} & \dots & -c_{1n_1} \\ 0 & \mu + c_{12} & -c_{23} + c_{13} & \dots & -c_{2n_1} + c_{1n_1} \\ 0 & -c_{32} + c_{12} & \mu + c_{13} & \dots & -c_{3n_1} + c_{1n_1} \\ \vdots & \vdots & \vdots & \vdots & \\ 0 & -c_{n_1 2} + c_{12} & -c_{n_1 3} + c_{13} & \dots & \mu + c_{1n_1} \end{vmatrix} \tag{16}$$

From equation (7), the sum of the i-th row in (16) is $\mu + c_{i1}$ for $i = 2, 3, \dots, n_1$. By subtracting columns $2, 3, \dots, n_1$ of determinant (16) from the first column, we obtain determinant (17).

$$|\mathbf{H}| = \begin{vmatrix} \mu & -c_{12} & -c_{13} & \dots & -c_{1n_1} \\ -\mu - c_{21} & \mu + c_{12} & -c_{23} + c_{13} & \dots & -c_{2n_1} + c_{1n_1} \\ -\mu - c_{31} & -c_{32} + c_{12} & \mu + c_{13} & \dots & -c_{3n_1} + c_{1n_1} \\ \vdots & \vdots & \vdots & \vdots & \\ -\mu - c_{n_1 1} & -c_{n_1 2} + c_{12} & -c_{n_1 3} + c_{13} & \dots & \mu + c_{1n_1} \end{vmatrix} \tag{17}$$

Add the first row of $|\mathbf{H}|$ to the rows $2, 3, \dots, n_1$, and we obtain determinant (18).

$$|\mathbf{H}| = \begin{vmatrix} \mu & -c_{12} & -c_{13} & \dots & -c_{1n_1} \\ -c_{21} & \mu & -c_{23} & \dots & -c_{2n_1} \\ -c_{31} & -c_{32} & \mu & \dots & -c_{3n_1} \\ \vdots & \vdots & \vdots & \vdots & \\ -c_{n_1 1} & -c_{n_1 2} & -c_{n_1 3} & \dots & \mu \end{vmatrix} \tag{18}$$

Then, we have

$$|\mathbf{A}| = \frac{1}{\mu - X}|\mathbf{H}| = \frac{1}{\mu - X}\Phi(\mathbf{C}'(G_1), \mu) \tag{19}$$

In a similar way, we can obtain

$$|\mathbf{B}| = \frac{1}{\mu - Y}|\mathbf{H}| = \frac{1}{\mu - Y}\Phi(\mathbf{C}'(G_2), \mu) \tag{20}$$

Substituting (19) and (20) back into (15) gives the result. □

Lemma 1 ([12]). *Let λ be an eigenvalue of square matrix $\mathbf{A}$, and $\mathbf{x}$ is its eigenvector. For any real number $k \neq 0$, $k\lambda$ be an eigenvalue of square matrix $k\mathbf{A}$ corresponding to the eigenvector $\mathbf{x}$.*

Theorem 2. *Let G_i be an r_i-regular graph of order n_i for $i = 1, 2$. Then, the ISI-energy of $G = G_1 + G_2$ is*

$$\varepsilon_{isi}(G) = \frac{r_1 + n_2}{r_1}\varepsilon_{isi}(G_1) + \frac{r_2 + n_1}{r_2}\varepsilon_{isi}(G_2) - \left(\frac{(n_2 + r_1)r_1}{2} + \frac{(n_1 + r_2)r_2}{2}\right)$$
$$+\frac{1}{2}\sqrt{((n_2 + r_1)r_1 - (n_1 + r_2)r_2)^2 + 16n_1 n_2\left(\frac{(n_1 + r_2)(n_2 + r_1)}{n_1 + n_2 + r_2 + r_1}\right)^2}$$

Proof. By Theorem 1, we have

$$\Phi(\mathcal{C}(G), \mu) = \frac{(\mu - X)(\mu - Y) - n_1 n_2 a^2}{(\mu - X)(\mu - Y)}\Phi(\mathcal{C}'(G_1), \mu)\Phi(\mathcal{C}'(G_2), \mu)$$

i.e.,

$$(\mu - X)(\mu - Y)\Phi(\mathcal{C}(G), \mu) = [(\mu - X)(\mu - Y) - n_1 n_2 a^2]\Phi(\mathcal{C}'(G_1), \mu)\Phi(\mathcal{C}'(G_2), \mu)$$

Let

$$P_1(\mu) = (\mu - X)(\mu - Y)\Phi(\mathcal{C}(G), \mu)$$

and

$$P_2(\mu) = [(\mu - X)(\mu - Y) - n_1 n_2 a^2]\Phi(\mathcal{C}'(G_1), \mu)\Phi(\mathcal{C}'(G_2), \mu).$$

It is obvious that the roots of $P_1(\mu) = 0$ are X, Y and the ISI-eigenvalues of $G_1 + G_2$. Hence, the sum of the absolute values of the roots of $P_1(\mu) = 0$ is $X + Y + \varepsilon_{isi}(G_1 + G_2)$.

The roots of $P_2(\mu) = 0$ are ISI-eigenvalues of $\mathcal{C}'(G_1)$ and $\mathcal{C}'(G_2)$ and

$$\frac{X + Y}{2} \pm \frac{1}{2}\sqrt{(X + Y)^2 - 4XY + 4n_1 n_2 a^2}.$$

It is easy to see that $\mathcal{C}'(G_1) = \frac{r_1+n_2}{r_1}\mathcal{C}(G_1)$, $\mathcal{C}'(G_2) = \frac{r_2+n_1}{r_2}\mathcal{C}(G_2)$. By Lemma 1, the sum of the absolute values of ISI-eigenvalues of $\mathcal{C}'(G_1)$ and $\mathcal{C}'(G_2)$ are

$$\frac{r_1+n_2}{r_1}\varepsilon_{isi}(G_1)$$

and

$$\frac{r_2+n_1}{r_2}\varepsilon_{isi}(G_2),$$

respectively.

Hence, the sum of the absolute values of the roots of $P_2(\mu) = 0$ is

$$\frac{r_1+n_2}{r_1}\varepsilon_{isi}(G_1) + \frac{r_2+n_1}{r_2}\varepsilon_{isi}(G_2)$$
$$+|\frac{X+Y}{2} - \frac{1}{2}\sqrt{(X+Y)^2 - 4XY + 4n_1n_2a^2}|$$
$$+|\frac{X+Y}{2} + \frac{1}{2}\sqrt{(X+Y)^2 - 4XY + 4n_1n_2a^2}|$$

Because $P_1(\mu) = P_2(\mu)$, we obtain

$$\begin{aligned}
\varepsilon_{isi}(G_1+G_2) &= \frac{r_1+n_2}{r_1}\varepsilon_{isi}(G_1) + \frac{r_2+n_1}{r_2}\varepsilon_{isi}(G_2) - (X+Y) \\
&+\left|\frac{X+Y}{2} - \frac{1}{2}\sqrt{(X+Y)^2 - 4XY + 4n_1n_2a^2}\right| \\
&+\left|\frac{X+Y}{2} + \frac{1}{2}\sqrt{(X+Y)^2 - 4XY + 4n_1n_2a^2}\right| \\
&= \frac{r_1+n_2}{r_1}\varepsilon_{isi}(G_1) + \frac{r_2+n_1}{r_2}\varepsilon_{isi}(G_2) - \frac{(r_1+n_2)r_1 + (r_2+n_1)r_2}{2} \\
&+\frac{1}{2}\sqrt{((r_1+n_2)r_1 - (r_2+n_1)r_2)^2 + 16n_1n_2\left(\frac{(r_1+n_2)(r_2+n_1)}{(r_1+n_2)+(r_2+n_1)}\right)^2}
\end{aligned}$$

which implies the required result.

This completes the proof. □

Corollary 1. *If $G_1, G_2, \ldots, G_k$, $k \geq 3$, are the ISI-equienergetic regular graphs of same order and of same degree, then $\varepsilon_{isi}(G_a + G_b) = \varepsilon_{isi}(G_c + G_d)$ for all $1 \leq a, b, c, d \leq k$.*

Corollary 2. *Let G_1 and G_2 be two ISI-noncospectral, ISI-equienergetic regular graphs of same order and of same degree. Then, for any regular graph H, $\varepsilon_{isi}(G_1 + H) = \varepsilon_{isi}(G_2 + H)$.*

The *complement* of a graph G is the graph $\overline{G}$ with vertex set $V(\overline{G}) = V(G)$ and two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in G [1].

The *line graph*, denoted by $L(G)$, of a graph G, is the graph with $V(L(G)) = E(G)$ and two vertices of $L(G)$ are connected by an edge if edges incident on it are adjacent in G. For $k = 1, 2, \ldots$, the k-th iterated line graph of G is defined as $L^k(G) = L(L^{(k-1)}(G))$, where $L^0(G) = G$ and $L^1(G) = L(G)$ [13].

Lemma 2 ([12]). *Let G be an n-vertex r-regular graph with the eigenvalues $r, \lambda_2, \ldots, \lambda_n$. Then, the eigenvalues of $\overline{G}$ are $n - r - 1, -\lambda_2 - 1, \ldots, -\lambda_n - 1$.*

Lemma 3 ([12])**.** *Let G be an n-vertex r-regular graph with the eigenvalues $r, \lambda_2, \ldots, \lambda_n$. Then, the eigenvalues of $L(G)$ are as follows*

$$\left.\begin{array}{cc} 2r-2 & and \\ \lambda_i + r - 2 & i = 2, \ldots, n \quad and \\ -2, & \frac{n(r-2)}{2} \quad times \end{array}\right\} \tag{21}$$

Take into account the graphs H_1 and H_2 as shown in Figure 1. Let $G_1 = L(H_1)$ and $G_2 = L(H_2)$ (see Figure 2). The characteristic polynomials of H_1 and H_2 are $\Phi(H_1, \lambda) = (\lambda - 3)\lambda^4(\lambda + 3)$ and $\Phi(H_2, \lambda) = (\lambda - 3)(\lambda - 1)\lambda^2(\lambda + 2)^2$, respectively.

On the basis of Lemma 3, we obtain the spectrums of G_1 and G_2 as

$$Spec(G_1) = \begin{pmatrix} 4 & 1 & -2 \\ 1 & 4 & 4 \end{pmatrix} \tag{22}$$

and

$$Spec(G_2) = \begin{pmatrix} 4 & 2 & 1 & -1 & -2 \\ 1 & 1 & 2 & 2 & 3 \end{pmatrix} \tag{23}$$

respectively. It is easy to see that $\varepsilon(G_1) = \varepsilon(G_2) = 16$.

Theorem 3. *For all $n \geq 9$, there exists a pair of connected ISI-noncospectral, ISI-equienergetic graphs of order n.*

Proof. Take into consideration the graphs G_1 and G_2 as shown in Figure 2. Graphs G_1 and G_2 are both connected 9-vertex 4-regular graphs. From (22), (23) and Lemma 1, we have $\varepsilon_{isi}(G_1) = \varepsilon_{isi}(G_2) = 2\varepsilon(G_1) = 32$, and $\varepsilon_{isi}(K_t) = (t-1)^2$.

Then, by Theorem 2, we have

$$\begin{aligned} \varepsilon_{isi}(G_1 + K_t) &= \varepsilon_{isi}(G_2 + K_t) \\ &= 6(t+4) + \frac{(t-1)(t+8)}{2} + \frac{1}{2}\sqrt{(t^2+3t-24)^2 + 36t\left(\frac{(t+8)(t+4)}{t+6}\right)^2}. \end{aligned}$$

Hence, $G_1 + K_t$ and $G_2 + K_t$ are two ISI-noncospectral and ISI-equienergetic graphs for all $n \geq 9$.

This completes the proof. □

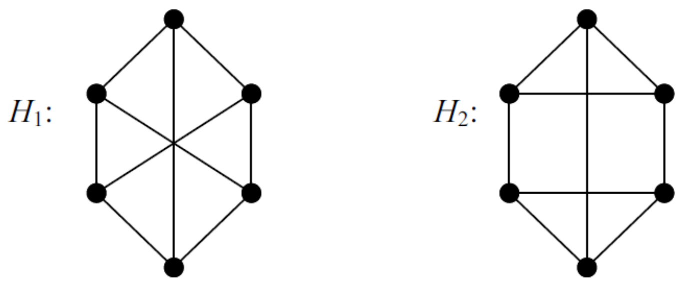

Figure 1. Two 3-regular graphs H_1 and H_2.

Lemma 4 ([14])**.** *Let G be an n-vertex $r(r \geq 3)$-regular graph. Then, among the positive eigenvalues of $\overline{L^2(G)}$, one is equal to the degree of $\overline{L^2(G)}$, whereas all others are equal to 1.*

Lemma 5 ([14])**.** *If G is an n-vertex and $r(r \geq 3)$-regular graph, then for $k \geq 2$, among the positive eigenvalues of $\overline{L^k(G)}$, one is equal to the degree of $\overline{L^k(G)}$, whereas all others are equal to 1.*

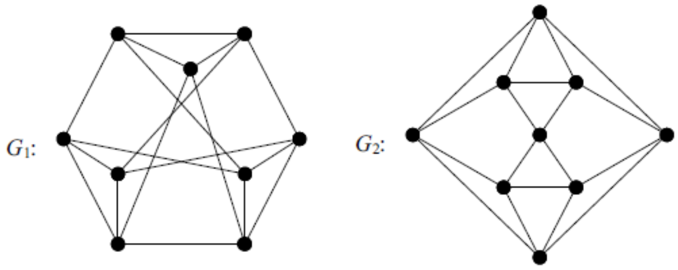

Figure 2. Two 4-regular ISI-equienergetic graphs G_1 and G_2.

Theorem 4. *If G is an n-vertex and $r(r \geq 3)$-regular graph, then*

$$\varepsilon_{isi}(\overline{L^2(G)}) = \frac{1}{4}(nr^2 - nr - 8r + 10)(2nr^2 - 3nr - 8r + 10).$$

Proof. If $\lambda, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of an n-vertex $r(r \geq 3)$-regular graph G, then by Lemma 3, the eigenvalues of $L(G)$ are

$$\left.\begin{array}{lll} 2r-2 & & and \\ \lambda_i + r - 2 & i = 2, \ldots, n & and \\ -2 & \frac{n(r-2)}{2} \ times & \end{array}\right\} \tag{24}$$

In view of the fact that $L(G)$ is a $\frac{nr}{2}$-vertex, $(2r-2)$-regular graph, from (24), the eigenvalues of $L^2(G)$ can be easily calculated as:

$$\left.\begin{array}{lll} \lambda_i + 3r - 6 & i = 1, 2, \ldots, n & and \\ 2r-6 & \frac{n(r-2)}{2} \ times & and \\ -2 & \frac{nr(r-2)}{2} \ times & \end{array}\right\} \tag{25}$$

Therefore, from Lemma 2, (24) and (25), we obtain the eigenvalues of $\overline{L^2(G)}$ as follows:

$$\left.\begin{array}{lll} -\lambda_i - 3r + 5 & i = 2, 3, \ldots, n & and \\ -2r + 5 & \frac{n(r-2)}{2} \ times & and \\ 1 & \frac{nr(r-2)}{2} \ times & and \\ \frac{nr(r-1)}{2} - 4r + 5 & & \end{array}\right\} \tag{26}$$

Hence, from Lemmas 1 and 4, the ISI-energy of $\overline{L^2(G)}$ is

$$\varepsilon_{isi}(\overline{L^2(G)}) = \frac{1}{2}(\frac{nr(r-1)}{2} - 4r + 5) \times 2[\frac{nr(r-1)}{2} - 4r + 5 + \frac{nr(r-2)}{2} \times 1]$$
$$= \frac{1}{4}(nr^2 - nr - 8r + 10)(2nr^2 - 3nr - 8r + 10).$$

This completes the proof. □

Theorem 5. *Let G_1 and G_2 be two n-vertex $r(r \geq 3)$-regular non-cospectral graphs. Then, $\overline{L^2(G_1)}$ and $\overline{L^2(G_2)}$ are ISI-noncospectral, ISI-equienergetic, and $\varepsilon_{isi}(\overline{L^2(G_1)}) = \varepsilon_{isi}(\overline{L^2(G_2)}) = \frac{1}{4}(nr^2 - nr - 8r + 10)(2nr^2 - 3nr - 8r + 10)$.*

Proof. The results can be easily obtained from Theorem 4. □

The line graph of an n_0-vertex r_0-regular graph G is a regular graph of order $n_1 = \frac{1}{2}r_0 n_0$ and of degree $r_1 = 2r_0 - 2$. Consequently, the order and degree of $L^k(G)$ are

$n_k = \frac{1}{2}r_{k-1}n_{k-1}$ and $r_k = 2r_{k-1} - 2$, where n_i and r_i denote the order and degree of $L^i(G)$ $(i = 0, 1, 2, \dots)$ [13]. Therefore,

$$r_k = 2^k r_0 - 2^{k+1} + 2 \tag{27}$$

and

$$n_k = \frac{n_0}{2^k}\prod_{i=0}^{k-1} r_i = \frac{n_0}{2^k}\prod_{i=0}^{k-1}(2^i r_0 - 2^{i+1} + 2) \tag{28}$$

Theorem 6. *If G is an n_0-vertex $r_0(r_0 \geq 3)$-regular graph, then for $k \geq 2$,*

$$\varepsilon_{isi}(\overline{L^k(G)}) = (n_k - r_k - 1)(\frac{2n_k r_k}{r_k + 2} - r_k - 1).$$

Proof. It is easily seen that $\overline{L^k(G)}$ is a regular graph of order n_k and degree $\frac{1}{2}r_{k-1}n_{k-1} - 2r_{k-1} + 1$. $\overline{L^k(G)}$ has $\frac{1}{2}n_{k-1}(r_{k-1} - 2)$ eigenvalues which are equal to 1. By Lemmas 1, 5 and the fact that the order and degree of $L^k(G)$ are $n_k = \frac{1}{2}r_{k-1}n_{k-1}$ and $r_k = 2r_{k-1} - 2$, we have

$$\begin{aligned}\varepsilon_{isi}(\overline{L^k(G)}) &= (\frac{1}{2}r_{k-1}n_{k-1} - 2r_{k-1} + 1)(r_{k-1}n_{k-1} - 2r_{k-1} - n_{k-1} + 1)\\ &= \frac{1}{4}(r_{k-1}n_{k-1} - 4r_{k-1} + 2)(2r_{k-1}n_{k-1} - 4r_{k-1} - 2n_{k-1} + 2)\\ &= (n_k - r_k - 1)(\frac{2n_k r_k}{r_k + 2} - r_k - 1).\end{aligned}$$

This completes the proof. □

Corollary 3. *If G is an n_0-vertex $r_0(r_0 \geq 3)$-regular graph, then*

$$\begin{aligned}\varepsilon_{isi}(\overline{L^k(G)}) = &\left([\frac{n_0}{2^k}\prod_{i=0}^{k-1}(2^i r_0 - 2^{i+1} + 2)] - 2^k r_0 + 2^{k+1} - 3\right)\\ &\times\left(\frac{[\frac{n_0}{2^k}\prod_{i=0}^{k-1}(2^i r_0 - 2^{i+1} + 2)](2^k r_0 - 2^{k+1} + 2)}{2^{k-1}r_0 - 2^k + 2} - 2^k r_0 + 2^{k+1} - 3\right)\end{aligned}$$

From Theorem 6 and Corollary 1, we see that for r_0-regular graph G of order n_0, the ε_{isi} of $\overline{L^k(G)})(k \geq 2)$ is fully determined by n_0 and r_0. Hence, we arrive at the following result.

Lemma 6. *Let G_1 and G_2 be two regular graphs of the same order and of the same degree. Then, for any $k \geq 1$, the following holds:*

(i) $\overline{L^k(G_1)}$ *and* $\overline{L^k(G_2)}$ *are of the same order and of the same size.*

(ii) $\overline{L^k(G_1)}$ *and* $\overline{L^k(G_2)}$ *are ISI-cospectral if and only if G_1 and G_2 are ISI-cospectral.*

Proof. Combining the fact that the number of edges of $L^k(G)$ is equal to the number of vertices of $L^{k+1}(G)$ and Equations (27) and (28), statement (i) holds. Statement (ii) can be obtained directly from Lemma 3.

This completes the proof. □

Theorem 7. *Let G_1 and G_2 be two non-cospectral regular graphs of the same order and of the same degree $r \geq 3$. Then, for any $k \geq 2$, graphs $\overline{L^k(G_1)}$ and $\overline{L^k(G_2)}$ are a pair of ISI-noncospectral and ISI-equienergetic graphs of equal order and of equal size.*

Corollary 3 provides a general method for constructing families of ISI-noncospectral, ISI-equienergetic graphs with the same order. In particular, from Theorem 3 and Theorem 3, it is easy to construct a pair of ISI-noncospectral, ISI-equienergetic n-vertex graphs for all $n \geq 9$.

Within Theorem 4, we obtained the expression in terms of n and r for the ISI-energy of the complement of the second iterated line graph of an n-ordered r-regular graph. Similar representations can be attained also for $\overline{L^k(G)}$, $k \geq 3$, i.e., the ISI-energy of the complement of the k-th iterated line graph, $k \geq 3$, of an n-ordered $r(r \geq 3)$-regular is also completely determined by the parameters n and r. In addition, for any $k > 2$, we can simply find a relevant collection of ISI-noncospectral and ISI-equienergetic regular graphs (of degree greater than 3) by constructing the complement of their k-th iterative line graph.

3. Conclusions

Graph energy has a very wide range of applications in the field of chemistry, physics, satellite communication, face recognition, crystallography, etc. It is worth noting that the energy of numerous graphs can be ascertained by making use of their ISI-energy. A notable discovery in graph energy theory is the existence of non-isomorphic and ISI-noncospectral graphs with equal ε_{isi}-values.

As far as we know, up to the present, researchers have not yet found a systematic approach to construct pairs (or larger families) of ISI-equienergetic graphs. Consequently, obtaining ISI-noncospectral but ISI-equienergetic graphs with the same order is an interesting and useful thing we should do. In this paper, by studying the ISI-characteristic polynomial of a join graph of two regular graphs, we construct pairs of connected, ISI-noncospectral, ISI-equienergetic graphs of order n for all $n \geq 9$. For example, we consider graph G_1, G_2 in Figure 2 and graph K_2. It is easy to obtain that $\varepsilon_{isi}(G_1) = \varepsilon_{isi}(G_2) = 32$, and $\varepsilon_{isi}(K_2) = 1$, then the ISI-energy of $G_1 + K_2$ and $G_2 + K_2$ are both equal to $\frac{82+\sqrt{4246}}{2}$, i.e., $G_1 + K_2$ and $G_2 + K_2$ are a pair of ISI-noncospectral, ISI-equienergetic 11-vertex graphs. In addition, for n-vertex $r(r \geq 3)$-regular graph G, and for each $k \geq 2$, we find $\varepsilon_{isi}(\overline{L^k(G)})$, depending solely on n and r. This result makes it possible to construct pairs of ISI-noncospectra same-order graphs having equal ISI-energies. For example, we consider graphs H_1 and H_2 as shown in Figure 1, it is easy to check that the ISI-spectrum of H_1 and H_2 are $\begin{pmatrix} \frac{9}{2} & 0 & -\frac{9}{2} \\ 1 & 4 & 1 \end{pmatrix}$ and $\begin{pmatrix} \frac{9}{2} & \frac{3}{2} & 0 & -\frac{6}{2} \\ 1 & 1 & 2 & 2 \end{pmatrix}$, respectively, i.e., H_1 and H_2 are ISI-noncospectral graphs. From Lemma 6, we know that $\overline{L^2(H_1)}$ and $\overline{L^2(H_2)}$ are also ISI-noncospectral graphs, and $\varepsilon_{isi}(\overline{L^2(H_2)}) = \varepsilon_{isi}(\overline{L^2(H_2)}) = 220$, i.e., $\overline{L^2(H_1)}$ and $\overline{L^2(H_2)}$, are a pair of ISI-noncospectral, ISI-equienergetic graphs. Furthermore, for any $k \geq 3$, by Lemma 6, we know that $\overline{L^k(H_1)}$ and $\overline{L^k(H_2)}$ are a pair of ISI-noncospectral, ISI-equienergetic graphs. Our results enable a systematic construction of pairs of ISI-noncospectral graphs of the same order, having equal ISI-energies.

The graph ISI-energy has taken its rise from theoretical chemistry. Trees, chemical trees, unicyclic and bicyclic graphs are common models of chemical structures. Thus, studying the ε_{isi} of these graphs, especially constructing ISI-noncospectral and ISI-equienergetic molecular graphs such as chemical trees, unicyclic, bicyclic and other useful graphs, is also an interesting research direction in the future.

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