Inverse sum indeg energy of graphs

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ABSTRACT Suppose $G$ is an $n$-vertex simple graph with vertex set $\{v_1, \ldots, v_n\}$ and $d_i$, $i = 1, \ldots, n$, is the degree of vertex $v_i$ in $G$. The ISI matrix $S(G) = [s_{ij}]_{n \times n}$ of $G$ is defined by $s_{ij} = \frac{d_i d_j}{d_i + d_j}$ if the vertices $v_i$ and $v_j$ are adjacent and $s_{ij} = 0$ otherwise. The $S$-eigenvalues of $G$ are the eigenvalues of its ISI matrix $S(G)$. Recently the notion of inverse sum indeg (henceforth, ISI) energy of graphs is introduced and is defined by $\sum_i |\tau_i|$, where $\tau_i$ are the $S$-eigenvalues. We give ISI energy formula of some graph classes. We also obtain some bounds for ISI energy of graphs. In the end we give some noncospectral equienergetic graphs with respect to inverse sum indeg energy.

INDEX TERMS Energy of graphs, inverse sum indeg energy, extremal bounds, equienergetic graphs.

I. INTRODUCTION

Topological indices predict many physio-chemical properties of chemical compounds. Among many discrete Adriatic indices, inverse sum indeg index was selected as a significant predictor of the total surface area of the octane isomers. Related to many topological indices, energy of a graph is defined and many of them have applications in chemistry. In this paper, we define inverse sum indeg energy of graphs related to the inverse sum indeg index of graphs. The energy of a graph determine the $\pi$-electron energy of a conjugated carbon molecule and energy of many types of graphs can be found by using inverse sum indeg energy of these graphs. Construction of equienergetic graphs is also an important direction in graph theory. Benefit of finding the equienergetic graphs is that one have to find the energy of only one graph in a class of all equienergetic graphs. This will ease the computation of a reader. A significant amount of research has been carried out in this direction.

A graph $G$ is a pair $G = (V(G), E(G))$, where $V(G)$ denotes the vertex set $\{v_1, \ldots, v_n\}$ and $E(G)$ denotes the edge set of $G$. The degree $d_i$ of a vertex $v_i$ is the number of edges incident on it. If vertices $v_i$ and $v_j$ are adjacent, we denote it by $v_i \sim v_j$. If vertices $v_i$ and $v_j$ are not adjacent, we denote it by $v_i \not\sim v_j$. An edge with end-vertices $v_i$ and $v_j$ is denoted by $v_iv_j$. A loop is an edge with same end-vertices. A graph is called simple if it has no loops and no two of its edges join the same pair of vertices. In the rest of paper, we consider simple graphs.

An $n$-vertex path $P_n$, $(n \geq 1)$, is a graph with vertex set $\{v_1, \ldots, v_n\}$ and edge set $\{v_jv_{j+1}| j = 1, 2, \ldots, n - 1\}$.

An $n$-vertex cycle $C_n (n \geq 3)$ is a graph with vertex set $\{v_1, \ldots, v_n\}$ and edge set $\{v_jv_{j+1}| j = 1, 2, \ldots, n - 1\} \cup \{v_nv_1\}$. Two graphs $G_1$ and $G_2$ are said to be isomorphic if there exists a bijection $\phi : V(G_1) \rightarrow V(G_2)$ such that $uv \in E(G_1)$ if and only if $\phi(u)\phi(v) \in E(G_2)$. We write $G_1 \cong G_2$ if $G_1$ and $G_2$ are isomorphic. The star graph $S_n$ of order $n$ is isomorphic to $K_{1,n-1}$. By $\overline{G}$, we denote the complement of $G$.

The adjacency matrix $A(G) = [a_{ij}]_{n \times n}$ of an $n$-vertex graph $G$ is defined as

$$a_{ij} = \begin{cases} 1 & \text{if } v_i \sim v_j, \\ 0 & \text{otherwise}. \end{cases}$$

The $A$-characteristic polynomial of $G$ is the polynomial

$$\Phi(G, \lambda) = \det(A(G) - \lambda I_n) = \lambda^n + \sum_{i=1}^{n} a_i \lambda^{n-i}.$$ 

where $I_n$ is the diagonal matrix of order $n$ with diagonal entries equal to 1. The $A$-eigenvalues of $G$ are the $A$-eigenvalues of $A(G)$. The spectrum of $G$, denoted by $\text{spec}_A(G)$, is the set of $A$-eigenvalues of $G$ together with their multiplicities.

The inverse sum indeg, (henceforth ISI) index, was studied in [24]. The ISI index is defined as

$$\text{ISI}(G) = \sum_{i,j} \frac{d_id_j}{d_i + d_j}.$$
Zangi et al. [26] defined the ISI matrix $S(G) = [s_{ij}]_{n \times n}$ of an $n$-vertex graph $G$ as:

$$s_{ij} = \begin{cases} \frac{d_id_j}{d_i + d_j} & \text{if } v_i \sim v_j, \\ 0 & \text{otherwise}. \end{cases}$$

The $S$-characteristic polynomial of $G$ is given by:

$$\Phi_S(G, \lambda) = \det(S(G) - \lambda I_n) = \lambda^n + \sum_{i=1}^{n} b_i \lambda^{n-i},$$

where $I_n$ is the diagonal matrix of order $n$ with diagonal entries equal to 1. The $S$-eigenvalues of $G$ are the $S$-eigenvalues of $S(G)$. The $S$-spectrum, $\text{spec}_S(G)$, of $G$, is the set of $S$-eigenvalues of $G$ together with their multiplicities. Since ISI matrix of graph is symmetric and real, therefore its eigenvalues are real. If $G$ is an $n$-vertex graph with distinct $S$-eigenvalues $\tau_1, \tau_2, \ldots, \tau_k$ and if their respective multiplicities are $p_1, p_2, \ldots, p_k$, we write the $S$-spectrum of $G$ as $\text{spec}_S(G) = \{\tau_1^{(p_1)}, \tau_2^{(p_2)}, \ldots, \tau_k^{(p_k)}\}$.

In 1978, the energy of a simple graph is defined by Gutman [11] as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. Many results on the graph energy can be found in literature. The concept of Randic energy is given by Bozkurt et al. [2], [3]. In 2014, Gutman et al. [12] gave some of the properties of Randic matrix and Randic energy. Sedlar et al. [23] study the properties of ISI index and finds extremal values of ISI index for some classes of graphs. Pattabiraman [17] gave some extremal bounds on ISI index. In 2018, Das et al. [8] summarized different types of energies of graphs introduced by many authors. Das et al. [8] find some of the lower and upper bounds for these energies of graphs. For recent results on different types of energies of graphs, one can study [6], [9], [10], [16], [18]–[21], [27].

Zangi et al. [26] introduce the concept of ISI energy of graphs. In this paper we obtain ISI energy formula of some well-known graphs. Upper and lower bounds are established. Finally, we give integral representation for ISI energy of graphs.

II. INVERSE SUM INDEG ENERGY

Let $\lambda_1, \ldots, \lambda_n$ be $A$-eigenvalues of an $n$-vertex graph $G$. Then Gutman [11] defined the energy of $G$ as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. Let $\tau_1, \ldots, \tau_n$ be the $S$-eigenvalues of $G$. Then Zangi et al. [26] define ISI energy of $G$ as

$$E_{ISI}(G) = \sum_{i=1}^{n} |\tau_i|.$$  

(II.2)

For convenience, we define some notations. We denote determinant of $S(G)$ by $\det(S(G))$. Let

$$Q = 2 \sum_{1 \leq i < j \leq n} \left( \frac{d_id_j}{d_i + d_j} \right)^2, \quad \Theta = \det(S(G)).$$

The trace of the matrix $S(G) = [s_{ij}]_{n \times n}$ is defined by $\sum_{i=1}^{n} s_{ii}$ and is denoted by $tr(S(G))$. Zangi et al. [26] prove the following lemma.

Lemma 2.1 (Zangi et al. [26]): Let $G$ be an $n$-vertex graph and let $\tau_1, \ldots, \tau_n$ be its $S$-eigenvalues. Then

(1) $\sum_{i=1}^{n} \tau_i = 0,$

(2) $tr(S^2(G)) = \sum_{i=1}^{n} \tau_i^2 = Q.$

Theorem 2.2: Let $G$ be an $n$-vertex simple and connected graph and let $m$ be the number of edges in $G$. Then

$$tr(S^2(G)) \leq tr(S^2(K_n)).$$

where the equality holds if and only if $G \cong K_n$.

Proof. First let $G \not\cong K_n$. Then $d_i \leq n - 1$ for every vertex $v_i$ of $G$, $i = 1, \ldots, n$. Therefore

$$\frac{d_id_j}{d_i + d_j} = \frac{1}{d_i + d_j} \leq \frac{1}{\frac{n-1}{n-1} + \frac{n-1}{n-1}} = \frac{n-1}{2},$$

$$tr(S^2(G)) = 2 \sum_{1 \leq i < j \leq n} \left( \frac{d_id_j}{d_i + d_j} \right)^2 \leq 2m \frac{(n-1)^2}{4} = \frac{m(n-1)^2}{2}.$$

As $G \not\cong K_n$, it holds that $m < \frac{n(n-1)}{2}$. Consequently

$$tr(S^2(G)) \leq \frac{m(n-1)^2}{2} < \frac{n(n-1)}{2} \times \frac{(n-1)^2}{2} = \frac{n(n-1)^3}{4}.$$

Now let $G \cong K_n$. Lemma 2.1 implies

$$tr(S^2(K_n)) = 2 \left( \frac{n(n-1)}{2} \times \frac{(n-1)^2}{4} \right) = \frac{n(n-1)^3}{4}.$$

Hence $tr(S^2(G)) \leq tr(S^2(K_n))$. This proves the result.

Suppose $G_1$ and $G_2$ are two graphs with disjoint vertex sets. Then the graph union $G_1 \cup G_2$ is a pair $G_1 \cup G_2 = \{V(G_1 \cup G_2), E(G_1 \cup G_2)\} = \{V(G_1 \cup V(G_2), E(G_1) \cup E(G_2))\}$. The degree of a vertex $v$ of $G_1 \cup G_2$ is equal to the degree of the vertex $v$ in the component $G_i$, $i = 1, 2$, that contains it. A square diagonal matrix whose diagonal elements are square matrices and the non-diagonal elements are 0 is called a block diagonal matrix.

Next theorem gives the relation between ISI energy of a graph and its components.

Theorem 2.3: Suppose $G_1, G_2, \ldots, G_s$ are the components of a graph $G$. Then $E_{ISI}(G) = \sum_{i=1}^{s} E_{ISI}(G_i)$.

Proof. Since $G_1, G_2, \ldots, G_s$ are the components of $G$, we can write $G = G_1 \cup G_2 \cup \cdots \cup G_s$. Then
$S(G)$ is a block diagonal matrix with diagonal elements $S(G_1), S(G_2), \ldots, S(G_s)$. Therefore

$$spec_S(G) = spec_S(G_1) \cup spec_S(G_2) \cup \cdots \cup spec_S(G_s).$$

Hence

$$E_{ISI}(G) = \sum_{i=1}^{k} E_{ISI}(G_i).$$

Following result follows directly from ISI matrix of $\overline{K_n}$.

**Lemma 2.4:** Suppose $G$ is an $n$-vertex graph. Then $E_{ISI}(G) = 0$ if and only if $G \cong \overline{K_n}$.

We now show that the ISI energy of a non-trivial graph, if it is an integer, must be an even positive integer.

**Theorem 2.5:** If $G \not\cong \overline{K_n}$ and the ISI energy of a graph $G$ is an integer then it must be an even positive integer.

Proof. Let $\tau_1, \ldots, \tau_n$ be $S$-eigenvalues of $G$ and with no loss of generality, assume that $\tau_1, \ldots, \tau_s$ are positive and $\tau_{s+1}, \ldots, \tau_n$ are non-negative. From Lemma 2.1, we have

$$\sum_{i=1}^{s} \tau_i + \sum_{i=s+1}^{n} \tau_i = \sum_{i=1}^{n} \tau_i = 0$$

This gives

$$\sum_{i=1}^{s} \tau_i = -\sum_{i=s+1}^{n} \tau_i.$$

Now

$$E_{ISI}(G) = \sum_{i=1}^{n} |\tau_i| = \sum_{i=1}^{s} \tau_i + \sum_{i=s+1}^{n} (-\tau_i) = 2\sum_{i=1}^{s} \tau_i.$$

Therefore ISI energy of $G$ is an even integer.

The distance between two vertices $v$ and $u$ of $G$ is the length of the shortest path between them. The maximum distance between a vertex $v$ to all other vertices of $G$ is called the eccentricity of $v$. The diameter of $G$ is the maximum eccentricity of any vertex in $G$. A matrix $M$ is irreducible if the digraph associated with $M$ is strongly connected. A matrix is non-negative if its all entries are non-negative.

In the following two results, we determine some properties of the $S$-eigenvalues. The idea of proof is taken from proof of Lemma 1.1 [7]

**Lemma 2.6:** Let $G$ be an $n$-vertex simple and connected graph. $n \geq 2$, with non-increasing $S$-eigenvalues $\tau_1 \geq \tau_2 \geq \cdots \geq \tau_n$. If $G$ has diameter at least 3, then $\tau_1 > \tau_2 \geq 0$. Proof. Since the graph $G$ is connected therefore $S(G)$ is an irreducible non-negative square matrix of order $n$. By Perron-Frobenius theorem, we have $\tau_1 > \tau_2$. Since $G$ has diameter at least 3, $P_4$ is the subgraph of $G$. Therefore we have $\tau_2(G) \geq \tau_2(P_4) = \frac{4}{3} > 0$, where $\tau_2(G)$ is the second largest $S$-eigenvalue of $G$ and $\tau_2(P_4)$ is the second largest $S$-eigenvalue of $P_4$. Hence $\tau_1 > \tau_2 > 0$.

**Lemma 2.7** (Brouwer and Haemers [4]): Let $G$ be a connected graph with greatest eigenvalue $\lambda_1$. Then $-\lambda_1$ is an eigenvalue of $G$ if and only if $G$ is bipartite.

**Theorem 2.8:** Suppose $G$ is an $n$-vertex graph, $n \geq 2$, with $S$-eigenvalues $\tau_1, \ldots, \tau_n$ and let its $A$-spectrum and $S$-spectrum are symmetric about the origin. Then $|\tau_1| = |\tau_2| = \cdots = |\tau_m| > 0 \ (m \geq 2)$ and the remaining $S$-eigenvalues are zero (if exist) if and only if $G \cong \bigcup_{j=1}^{p} K_{r,s}$, where $p(r + s) = n$ and one of the $r$ or $s$ is greater than 1.

Proof. First assume that

$$|\tau_1| = |\tau_2| = \cdots = |\tau_m| > 0 \ (m \geq 2) \quad (II.3)$$

and the remaining $S$-eigenvalues are zero (if exist). Then each component of $G$ has atmost three distinct $S$-eigenvalues. Let $H$ be a component of $G$. From equation (II.3) and Lemma 2.7, we see that $H$ is bipartite. If $H$ is not a complete bipartite graph, then the diameter of $H$ is at least 3. Therefore by Lemma 2.6 and equation (II.3), we get a contradiction. Hence $H$ is a complete bipartite graph.

As $H$ is arbitrary component of $G$, therefore $G \cong \bigcup_{j=1}^{p} K_{r,s}$, where $p(r + s) = n$.

The converse statement is easy to prove.

### III. ISI ENERGY OF SOME GRAPHS

In this section, we prove ISI energy formulae for some classes of graphs.

The $A$-spectrum of $K_n$ and $K_{m,n}$ is given by

$$spec_A(K_n) = \{(-1)^{n-1}, (n-1)\},$$

$$spec_A(K_{m,n}) = \{(0)^{m+n-2}, \pm \sqrt{mn}\}$$

Bhat and Pirzada [1] gave the following energy formula for cycle $C_n$ of order $n$:

$$E(C_n) = \begin{cases} 4 \cot \frac{\pi}{n} & \text{if } n \equiv 0(\text{mod}4) \\ 4 \csc \frac{\pi}{n} & \text{if } n \equiv 2(\text{mod}4) \\ 2 \csc \frac{\pi}{2n} & \text{if } n \equiv 1(\text{mod}2). \end{cases} \quad (III.4)$$

A graph whose vertices have equal degree is called a regular graph. A regular graph whose vertices have degree $k$ is called a $k$-regular graph. Zangi et al. [26] prove the following result.

**Theorem 3.1** (Zangi et al. [26]): Suppose $G$ is an $n$-vertex $k$-regular graph. Then $E_{ISI}(G) = \frac{k}{2} E(G)$.

Using Theorem 3.1, we get the following results.

**Theorem 3.2:** $E_{ISI}(C_n) = E(C_n)$

**Theorem 3.3:** $E_{ISI}(K_n) = (n - 1)^2$.

**Remark 3.4:** Let $n \equiv 2(\text{mod} 4)$. Then from equation (III.4), one can see that $E_{ISI}(C_n) = 2E_{ISI}(C_{\frac{n}{2}})$. 

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Now we obtain the ISI energy formula for complete bipartite graph.

**Theorem 3.5:** \( E_{\text{ISI}}(K_{m,n}) = \frac{2(mn)^{\frac{3}{2}}}{m+n} \).

Proof. Let \( B \) be an \( m \times n \) matrix and \( C \) be an \( n \times m \) matrix, where all entries of \( B \) and \( C \) are equal to \( \frac{mn}{m+n} \). Let \( O \) be a zero matrix of order \( m \times m \) and \( O' \) be a zero matrix of order \( n \times n \). Then

\[
S(K_{m,n}) = \begin{bmatrix} O & B \\ C & O' \end{bmatrix}.
\]

That is,

\[
S(K_{m,n}) = \frac{mn}{m+n}A(K_{m,n}).
\]

Hence

\[
\text{spec}_G(K_{m,n}) = \left\{ \frac{(mn)^{\frac{3}{2}}}{m+n}, 0^{(m+n-2)}, \frac{(mn)^{\frac{3}{2}}}{m+n} \right\}.
\]

Therefore

\[
E_{\text{ISI}}(K_{m,n}) = \sum_{j=1}^{m+n} |\tau_j| = \left\lfloor \frac{(mn)^{\frac{3}{2}}}{m+n} \right\rfloor + \left\lfloor \frac{(mn)^{\frac{3}{2}}}{m+n} \right\rfloor = \frac{2(mn)^{\frac{3}{2}}}{m+n}.
\]

The proof is complete.

Following corollary is an easy consequence of Theorem 3.5.

**Corollary 3.5.1:** \( E_{\text{ISI}}(S_n) = \frac{2(n-1)^{\frac{3}{2}}}{n} \).

**Remark 3.6:** By Theorem 2.3 and Theorem 3.3, it is easily seen that \( E_{\text{ISI}}(\overrightarrow{K}_{m,n}) = m^2 - n^2 - 2(m+n-1) \).

Let \( A = (a_{ij}) \) be the square matrix of order \( p \) with eigenvalues \( \lambda_k \) and \( B \) be the square matrix of order \( q \) with eigenvalues \( \beta_i \), \( i, j, k = 1, \ldots, p, l = 1, \ldots, q \). The Kronecker product \( A \otimes B \) of matrices \( A \) and \( B \) is the matrix obtained by replacing each entry \( a_{ij} \) of \( A \) by \( a_{ij} B \). The eigenvalues of \( A \otimes B \) are \( \lambda_k \beta_l \).

Let \( G \) be a graph with vertex set \( V(G) \) and let \( V' \) be the copy of \( V(G) \) such that \( V(G) \cap V' = \emptyset \) and \( g : V(G) \rightarrow V' \) is a bijection. For \( u \in V(G) \), we write \( g(u) = u' \).

The duplication of a graph \( G \), denoted by \( G^* \), is the graph with vertex set \( V(G) \cup V' \) whose edges are as follows: In a graph \( G \), \( uv \in E(G) \) if and only if \( uv \in E(G^*) \) and \( vu' \in E(G^*) \).

Let \( G \) be an \( n \)-vertex graph with vertex set \( V(G) \), and let \( H_1, \ldots, H_d \) be the \( d \) copies of \( G \) with vertex sets \( V_i(H_1), \ldots, V_i(H_d) \) and let \( V_i(H_i) = \{ v_{i1}, \ldots, v_{in} \} \), \( i = 1, \ldots, d \) and \( v_{ij} \) denotes the \( j \)-th vertex of the \( i \)-th copy of \( G \), \( j = 1, \ldots, n \). The \( d \)-double graph \( G^d \) of a graph \( G \) is the graph with vertex set \( V_1(H_1) \cup \cdots \cup V_d(H_d) \) whose edges are as follows: In a graph \( G \), \( v_1v_2 \in E(G) \) if and only if \( v_1v_2k \in E(G^d) \) with \( i \neq k \) and \( k = 1, \ldots, d \). See Figure 1.

**FIGURE 1.** \( P_3 \) and its 2-double graph \( P_3^2 \)

Now we give the relation of ISI energy of graph \( G \) with ISI energy of its duplication graph and \( d \)-double graph.

**Theorem 3.7:** Let \( G \) be an \( n \)-vertex graph. Then \( E_{\text{ISI}}(G^*) = 2E_{\text{ISI}}(G) \).

Proof. Let \( O \) be an \( n \times n \) matrix. By proper labelling of the vertices and by the definition of \( G^* \), we get

\[
S(G^*) = \begin{bmatrix} O & S(G) \\ S(G) & O \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes S(G).
\]

Thus the spectrum of \( S(G^*) \) is \( \pm \tau_i, i = 1, \ldots, n \). Hence \( E_{\text{ISI}}(G^*) = 2E_{\text{ISI}}(G) \).

**Theorem 3.8:** Let \( G \) be an \( n \)-vertex graph. Then \( E_{\text{ISI}}(G^{**}) = d^2E_{\text{ISI}}(G) \).

Proof. Let \( J_d \) be a \( d \times d \) matrix whose every entry is equal to \( 1 \). By proper labeling of the vertices and by the definition of \( G^d \), we have

\[
S(G^d) = \begin{bmatrix} dS(G) & dS(G) & \cdots & dS(G) \\ dS(G) & dS(G) & \cdots & dS(G) \\ \vdots & \vdots & \ddots & \vdots \\ dS(G) & dS(G) & \cdots & dS(G) \end{bmatrix}_{dn \times dn}
\]

Therefore \( S(G^d) = d \times (S(G) \otimes J_d) \), where \( A \)-spectrum of \( J_d \) is \( d \) with multiplicity \( 1 \) and \( 0 \) with multiplicity \( d-1 \). By property of Kronecker product of matrices, the \( S \)-spectrum of \( G^d \) is \( 0 \) with multiplicity \( d-1 \) and \( S \)-spectrum of \( G \). Therefore we get \( E_{\text{ISI}}(G^{**}) = d^2E_{\text{ISI}}(G) \).

**IV. BOUNDS AND INTEGRAL REPRESENTATION FOR ISI ENERGY**

In this section, we give some bounds for the ISI energy of graphs.

Let \( B \) be a matrix of order \( n \times n \) such that \( b_{ij} = 0 \) if \( v_i \not\sim v_j \) and \( b_{ij} = F(d_i, d_j) \) if \( v_i \sim v_j \), where \( F \) is the function with the property \( F(y, z) = F(z, y) \). Das et al. [8] prove the following theorem for eigenvalues of degree based energies of graphs.
Theorem 4.1 (Das et al. [8]): For the eigenvalues \( f_1 \geq f_2 \geq \cdots \geq f_n \) of a matrix \( M \), the following inequalities hold.

\[
\sqrt{\frac{\text{tr}(B^2)}{n(n-1)}} \leq f_1 \leq \sqrt{\frac{(n-1) \text{tr}(B^2)}{n}},
\]
\[
-\sqrt{\frac{(n-1) \text{tr}(B^2)}{n}} \leq f_n \leq \sqrt{\frac{(n-1) \text{tr}(B^2)}{n}},
\]
\[
-\sqrt{\frac{(k-1) \text{tr}(B^2)}{n(n-k+1)}} \leq f_k \leq \sqrt{\frac{(n-k) \text{tr}(B^2)}{kn}},
\]

for \( k = 2, \ldots, n-1 \).

The following result is obtained by using Theorem 4.1.

Theorem 4.2: For the eigenvalues \( \tau_1 \geq \tau_2 \geq \cdots \geq \tau_n \) of \( S(G) \), the following inequalities hold.

\[
\sqrt{\frac{Q}{n(n-1)}} \leq \tau_1 \leq \sqrt{\frac{(n-1) Q}{n}},
\]
\[
-\sqrt{\frac{(n-1) Q}{n}} \leq \tau_n \leq -\sqrt{\frac{Q}{n(n-1)}},
\]
\[
-\sqrt{\frac{(k-1) Q}{n(n-k+1)}} \leq \tau_k \leq \sqrt{\frac{(n-k) Q}{kn}},
\]

for \( k = 2, \ldots, n \).

Using Theorem 2.2 and Theorem 4.2, we get the following result for an \( n \)-vertex connected graph \( G \).

Theorem 4.3: For \( S \)-eigenvalues \( \tau_1 \geq \tau_2 \geq \cdots \geq \tau_n \) of a connected graph \( G \), the following inequalities hold.

\[
\sqrt{\frac{Q}{n(n-1)}} \leq \tau_1 \leq E_{ISI}(K_n),
\]
\[
-E_{ISI}(K_n) \leq \tau_n \leq -\sqrt{\frac{Q}{n(n-1)}},
\]
\[
-\sqrt{\frac{(k-1) (n-1)^3}{4(n-k+1)}} \leq \tau_k \leq \sqrt{\frac{(n-k) (n-1)^3}{4k}},
\]

for \( k = 2, \ldots, n-1 \).

In next theorem, we find bounds for ISI energy in terms of trace of matrix \( S^2(G) \) and determinant of \( S(G) \).

Theorem 4.4: Let \( G \) be an \( n \)-vertex simple graph, \( n \geq 2 \). Then

\[
n|\Theta|^{\frac{2}{n}} \leq E_{ISI}(G) \leq \sqrt{nQ},
\]

where \( \Theta = \text{det } S(G) \)

Proof. As we know that arithmetic mean is always less than quadratic mean, therefore

\[
E_{ISI}(G) = \sum_{i=1}^{n} |\tau_i| \leq \sqrt{n \sum_{i=1}^{n} |\tau_i|^2} \leq \sqrt{n Q}.
\]

Quadratic-Geometric mean inequality gives,

\[
(E_{ISI}(G))^2 = \left( \sum_{i=1}^{n} |\tau_i| \right)^2 \geq \sum_{i=1}^{n} |\tau_i|^2 \geq n (\prod_{i=1}^{n} |\tau_i|)^{\frac{2}{n}} = n |\Theta|^{\frac{2}{n}}.
\]

The proof is complete.

Now we have the following theorem. The proof is same as the proof of Theorem 3 [8] and is thus excluded.

Theorem 4.5: Let \( G \) be a simple \( n \)-vertex graph with \( n \geq 2 \) vertices. Then

\[
\sqrt{Q + n(n-1)} |\Theta|^{\frac{2}{n}} \leq E_{ISI}(G) \leq \sqrt{(n-1) Q + n |\Theta|^{\frac{2}{n}}}.
\]

In Theorem 4.6, we obtain bounds for ISI energy in terms of the number of edges, minimum and maximum degrees of a simple graph.

Theorem 4.6: Suppose \( G \) is an \( n \)-vertex simple graph with \( m \) edges, minimum degree \( \delta \) and maximum degree \( \Delta \). Then

\[
E_{ISI}(G) \geq \sqrt{\frac{m \delta^2 + n(n-1)}{2} |\Theta|^{\frac{2}{n}}},
\]
\[
E_{ISI}(G) \leq \sqrt{\frac{m(n-1) \Delta^2}{2} + n |\Theta|^{\frac{2}{n}}}.
\]

Proof. For each vertex \( v_i \) of \( G \), \( \delta \leq d_i \leq \Delta \), \( i = 1, 2, \ldots, n \). Using this fact, we get

\[
\frac{1}{d_i} + \frac{1}{d_j} \leq \frac{1}{\delta} + \frac{1}{\Delta} = \frac{\Delta}{2},
\]
\[
\frac{1}{d_i} + \frac{1}{d_j} \geq \frac{1}{\delta} + \frac{1}{\Delta} = \frac{\delta}{2}.
\]

Hence

\[
Q = 2 \sum_{1 \leq i < j \leq n} \left( \frac{d_i d_j}{d_i + d_j} \right)^2 \leq 2m \frac{\Delta^2}{4} = \frac{m \Delta^2}{2},
\]
\[
Q = 2 \sum_{1 \leq i < j \leq n} \left( \frac{d_i d_j}{d_i + d_j} \right)^2 \geq 2m \frac{\delta^2}{4} = \frac{m \delta^2}{2}.
\]

Now using Theorem 4.5, we obtain the desired result.
Coulson [5] prove the following integral representation of energy of graphs.

**Theorem 4.7 (Coulson [5]):** Let $G$ be an $n$-vertex simple graph, then

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left( n - i\lambda \Phi'(G, i\lambda) \right) d\lambda,$$

where $\Phi'(G, \lambda) = \frac{d}{d\lambda} \Phi(G, i\lambda)$ and $i = \sqrt{-1}$.

Next theorem is an analogue of Theorem 4.7.

**Theorem 4.8:** Let $G$ be a simple graph of order $n$. Then

$$E_{ISI}(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left( n - i\lambda \Phi'(S, i\lambda) \right) d\lambda,$$

where $\Phi'(S, \lambda) = \frac{d}{d\lambda} \Phi(S, i\lambda)$ and $i = \sqrt{-1}$.

**Corollary 4.8.1:** If $G$ is an $n$-vertex graph then

$$E_{ISI}(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{\lambda^2} \ln \left( \lambda^2 \Phi(S, i\lambda) \right).$$

The following result is similar to the graph energy.

**Theorem 4.9:** Let $G$ be an $n$-vertex graph with $S$-characteristic polynomial $\Phi(S, \lambda) = \lambda^n + \sum_{i=1}^{n} b_i \lambda^{n-i}$. Then

$$E_{ISI}(G) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\lambda^2} \log \left( \left( \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i b_{2i}(G) \lambda^{2i} \right)^2 + \left( \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i b_{2i+1}(G) \lambda^{2i+1} \right)^2 \right) d\lambda.$$

Now we give the following result based on numerical testing. The application of Coulson-type integral expressions for proving the conjecture was (so far) not successful.

**Conjecture 4.10:** Among all $n$-vertex trees, the tree with minimal ISI energy is $S_n$ and the tree with maximal ISI energy is $P_n$.

## V. S-EQUIENERGETIC GRAPHS

Two graphs with same $S$-spectrum are said to be $S$-cospectral, otherwise $S$-noncospectral. Two $S$-equienergetic graphs are the graphs which have same ISI energy. Two isomorphic graphs are always $S$-equienergetic and thus are $S$-equienergetic. We construct few classes of $S$-noncospectral $S$-equienergetic graphs.

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 $G$.

Let $G$ be a $k$-regular $n$-vertex graph. Let $L_i(G) = L(G), L_i(G) = L(L_{i-1}(G)), i = 1, 2, \ldots$ be the iterated line graphs of $G$. Ramane et al. [22] prove the following energy formula for $L_2(G)$.

$$E(L_2(G)) = 2nk(k-2). \quad (V.5)$$

**Theorem 5.1:** Suppose $G_1$ and $G_2$ are two $k$-regular $n$-vertex $A$-noncospectral graphs. Then $L_2(G_1)$ and $L_2(G_2)$ are $S$-noncospectral $S$-equienergetic graphs.

Proof. If $G$ is an $n$-vertex $k$-regular then $L_2(G)$ is $\frac{1}{2}nk(k-1)$-vertex $(4k-6)$-regular graph. By Theorem 3.1 and equation (V.5), we get

$$E_{ISI}(L_2(G)) = (2k-3)E(L_2(G)) = 2nk(k-3)(k-2).$$

Hence $E_{ISI}(L_2(G_1)) = E_{ISI}(L_2(G_2)).$

Since $S(L_2(G)) = (2k-3)A(L_2(G))$ and $L_2(G_1)$ and, $L_2(G_2)$ are $A$-noncospectral graphs, therefore $L_2(G_1)$ and $L_2(G_2)$ are also $S$-noncospectral graphs.

**Corollary 5.1.1:** Suppose $G_1$ and $G_2$ are two $k$-regular $n$-vertex $A$-noncospectral graphs. Then for any $m \geq 2$, $L_m(G_1)$ and $L_m(G_2)$ are $S$-noncospectral $S$-equienergetic.

**Theorem 5.2:** Suppose $G_1$ and $G_2$ are two $n$-vertex $S$-noncospectral $S$-equienergetic graphs. Then $G_1 \cup \overline{K}_r$ and $G_2 \cup \overline{K}_r$ are $S$-noncospectral $S$-equienergetic.

Proof. By Theorem 2.3, we have

$$E_{ISI}(G_1 \cup \overline{K}_r) = E_{ISI}(G_1) + E_{ISI}(\overline{K}_r) = E_{ISI}(G_2) + E_{ISI}(\overline{K}_r) = E_{ISI}(G_2 \cup \overline{K}_r).$$

Since $G_1$ and $G_2$ are $S$-noncospectral, therefore $G_1 \cup \overline{K}_r$ and $G_2 \cup \overline{K}_r$ are $S$-noncospectral.

**Corollary 5.2.1:** Suppose $G_1$ and $G_2$ are two $k$-regular $n$-vertex $A$-noncospectral graphs. Then for any $m \geq 2$, $L_m(G_1) \cup \overline{K}_r$ and $L_m(G_2) \cup \overline{K}_r$ are $S$-noncospectral $S$-equienergetic.

The following two theorems give some more classes of $S$-equienergetic graphs.

**Theorem 5.3:** Let $G$ be any $n$-vertex graph and $d \equiv 0 \pmod 2$. Also let $\hat{G}$ be the graph which is the union of $\frac{d^2}{2}$ copies of $G^*$. Then $E_{ISI}(G^d) = E_{ISI}(\hat{G})$.

Proof. By definition of $\hat{G}$ and proof of Theorem 2.3, it is easy to see that $S(G)$ is a block diagonal matrix with diagonal elements $S(G^*)$ and $S$-spectrum of $\hat{G}$ is $\pm \tau_i$ each with multiplicity $\frac{d^2}{2}, i = 1, \ldots, n$. Also in proof of Theorem 3.8, we see that the $S$-spectrum of $G^d$ is 0 with multiplicity $d-1$ and $d^3 \tau_i, i = 1, \ldots, n$. Therefore $\hat{G}$ and $G^d$ are $S$-noncospectral and $S$-equienergetic graphs.

**Theorem 5.4:** Let $G$ be an $n$-vertex graph whose at least one component is cycle of some order. Let $H$ be another $n$-vertex graph with same components as of $G$ except for the component which is cycle. Corresponding to each cycle (say $C_m$) in $G$, where $m \equiv 2 \pmod 4$, the graph $H$ has two cycles of half the order of $C_m$ (say $C_{m'}$). Then $G$ and $H$ are $S$-noncospectral and $S$-equienergetic graphs.

Proof. The result follows from Theorem 2.3 and Remark 3.4.

## VI. CONCLUSION

The energy of a graph has wide range of applications in chemistry. Energy of many types of graphs can be found by using inverse sum indeg energy of those graphs. In this paper...
we present some properties of ISI energy and S-spectra of graphs. We also find relation of ISI energy of some special types of graphs with graph energy. In future, finding graphs with extremal ISI energy in class of trees, chemical trees, unicyclic graphs, bicyclic graphs and in another graph classes will be an interesting and a challenging problem.

REFERENCES


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