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MINIMUM PENDANT DOMINATING ESTRADA INDEX OF A GRAPH

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Abstract. The main purpose of this paper is to introduce the concept of minimum pendant dominating Estrada index of a graph. First, we compute minimum pendant dominating Estrada index for complete graph, star graph, complete bipartite graph and cocktail party graph which are amongst the most widely-used graph classes. Also, upper and lower bounds for this new index are established. Finally, the relations between the new Estrada index and the new type of energy are investigated.

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1. Introduction

Let G be a simple, finite, undirected graph with vertex set $V(G)$ and edge set $E(G)$. Let the n vertices of G be labeled by $v_1, v_2, \cdots, v_n$. Two vertices v_i and v_j are said to be adjacent if $v_iv_j \in E(G)$. The degree of a vertex $v_i \in V(G)$ is the number of vertices adjacent to v_i and is denoted by $d_G(v_i)$. A walk is a sequence of vertices and edges of the graph. A graph is connected if each pair of vertices in a graph is joined by a walk. A bipartite graph is a graph such that its vertex set can be partitioned into two sets X and Y (called the partite sets) such that every edge meets both X and Y. A complete bipartite graph is a bipartite graph such that any vertex of a partite set is adjacent to all vertices in the other partite set. A complete bipartite graph with partite sets of cardinalities p and q is denoted by $K_{p,q}$. The graph $K_{1,n-1}$ is also called a star graph of order n, denoted by S_n. A simple connected undirected graph in which every pair of distinct vertices is connected by a unique edge is called a complete graph and is denoted by K_n. The *adjacency* matrix of a graph G is a square matrix $A(G) = [a_{ij}]$ of order n, defined via

$$a_{ij} = \begin{cases} 1 & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent} \\ 0 & \text{otherwise.} \end{cases}$$

The eigenvalues of $A(G)$ are the adjacency eigenvalues of G, and they are labeled by $\lambda_1, \lambda_2, \cdots, \lambda_n$. The notion of graph energy is a graph-spectrum-based quantity introduced in the 1970s. After a latent period of 20-30 years, it became a popular research topic both in mathematical chemistry and in pure spectral graph theory, resulting over a thousand published papers. The graph energy was defined by Gutman as the sum of absolute values of the eigenvalues of the adjacency matrix of a graph G, namely as

$$E = \sum_{i=1}^{n} | \lambda_i | . \tag{1}$$

This concept was intensively studied in chemistry since it can be used to approximate the total π-*electron* energy of a molecule (see, e.g. [21, 22]). Since then, mathematical properties of energy were also discovered (see e.g. [4, 7], [26]-[28]).

In spectral graph theory, the eigenvalues of several matrices like adjacency matrix, Laplacian matrix, distance matrix, Zagreb matrices, etc. are studied extensively for more than 50 years. Recently, maximum degree matrix, minimum degree matrix and adjacency matrix with respect to a subset S of $V(G)$ of a graph G are introduced and studied in [1, 2, 3, 32].

A graph-spectrum-based graph invariant was introduced by Estrada [12, 13], which was defined by

$$EE = EE(G) = \sum_{i=1}^{n} e^{\lambda_i}.$$

EE is nowadays usually referred to as the Estrada index, see [30]. Although invented only a few years ago, [12], the Estrada index has already found numerous applications. It was used to quantify the degree of folding of long-chain molecules, especially proteins, [13]. Another fully unrelated application of EE (this time for simple graphs, like those studied in the present paper) was put forward by Estrada and Rodríguez-Velázquez, [18, 19]. They showed that EE provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. These ideas were recently further elaborated and extended in [15]. In [20], a connection between EE and the concept of extended atomic branching was established, which was an attempt to apply EE in quantum chemistry. Another such application, this time in statistical thermodynamics, was proposed by Estrada and Hatano, [17], and later further extended in [16]. There are also applications in biochemical, [14], physico–chemical, [20], and network-theoretical studies, [18, 19]. In addition, this graph invariant is taken the attention of mathematicians as well. Indeed, in the last few years, quite a few mathematicians became interested in the Estrada index and communicated mathematical results on EE in mathematical journals. In what follows, we briefly survey the most significant ones of these results. Some mathematical properties of the Estrada index were established in [8, 9, 10, 23, 24, 25]. One of the most important properties is the following:

$$EE = \sum_{k=1}^{\infty} \frac{M_k(G)}{k!}$$

where $M_k = M_k(G)$ is the k-th moment of a graph G. We get $M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k$. It is well-known that $M_k(G)$ is equal to the number of closed walks of length k in G.

Recently, the analogous variants of this index such as the distance Estrada index, [6], the Seidel-Estrada index, [5], and the Harary energy and Harary Estrada index of a graph, [29], were introduced. Bearing this in mind, it seems to be purposeful to consider also the graph Estrada indices pertaining the minimum dominating number. Relatedly, we would have to introduce the minimum pendant dominating Estrada indices.

This paper is organized as follows: In Section 2, we give a list of some previously known results. In Section 3, after introducing the minimum pendant dominating Estrada index, we establish upper and lower bounds for it. In Section 4, we investigate relations between the minimum pendant dominating Estrada index and the minimum pendant dominating energy.

2. Preliminaries and known results

In this section, we shall list some previously known results that will be needed in the next sections. First, we recall a definition:

Definition 2.1. *(cf. [31]) The cocktail party graph denoted by $K_{n\times 2}$ is a graph having the vertex set $V = \bigcup_{i=1}^{n}\{u_i, v_i\}$ and the edge set $E = \{u_iu_j, v_iv_j : i \neq j\} \bigcup \{u_iv_j, v_iu_j : 1 \leqslant i < j \leqslant n\}$.*

The following two properties can be found in any calculus book:

Remark 2.1. *For any real x, the power series expansion of e^x is as follows:*

$$e^x = \sum_{k\geqslant 0} \frac{x^k}{k!}. \tag{2}$$

Remark 2.2. *For non-negative $x_1, x_2, \cdots, x_n$ and $k \geqslant 2$,*

$$\sum_{i=1}^{n} {x_i}^k \leqslant (\sum_{i=1}^{n} {x_i}^2)^{\frac{k}{2}}. \tag{3}$$

3. The minimum pendant dominating Estrada index

In this section, we consider the minimum pendant dominating Estrada index of a graph G. Also we present lower and upper bounds for it.

Let G be a simple graph having n vertices. Let G have the vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$ and edge set $E(G)$. A subset D of $V(G)$ is called a dominating set of G if every vertex of $V(G) - D$ is adjacent to some vertex in D. Any dominating set with minimum cardinality is called a minimum dominating set and its cardinality will be denoted by $\gamma(G)$. A dominating set D is called a pendant dominating set if D contains at least one pendant vertex, that is, a vertex of degree 1. The least cardinality of a pendant dominating set in G is called the pendant domination number of G denoted by $\gamma_{pe}(G)$, (see, for details, [31]). The minimum pendant dominating matrix of G, [31], is the $n \times n$ matrix defined by $A_{pe,D}(G) := (\mathbf{a}_{ij})$ where

$$\mathbf{a}_{ij} = \begin{cases} 1 & \text{if } v_iv_j \in E(G) \\ 1 & \text{if } \ i = j \text{ and } \ v_i \in D \\ 0 & \text{otherwise.} \end{cases}$$

The minimum pendant dominating eigenvalues of the graph G are the eigenvalues of $A_{pe}(G)$. Since $A_{pe}(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order as $\alpha_1 \geqslant \alpha_2 \geqslant \cdots \geqslant \alpha_n$. The minimum pendant dominating energy of G is defined to be the sum of the absolute values of the eigenvalues of $E_{pe}(G)$. In symbols, we write

$$E_{pe}(G) := \sum_{i=1}^{n} |\alpha_i|,$$

(cf. [31]). Bearing this in mind, we would have to introduce the minimum pendant dominating Estrada index of a graph as follows:

Definition 3.1. *Let G be a graph having n vertices and let the eigenvalues of its minimum pendant dominating matrix be $\alpha_1 \geqslant \alpha_2 \geqslant \cdots \geqslant \alpha_n$. Then the minimum pendant dominating Estrada index of G, denoted by $EE_{pe}(G)$, is defined to be*

$$EE_{pe}(G) = \sum_{i=1}^{n} e^{\alpha_i}.$$

Then

$$EE_{pe}(G) = \sum_{k=1}^{\infty} \frac{R_k}{k!}$$

where

$$R_k(G) = \sum_{i=1}^{n} \alpha_i^k.$$

It is clear from the below example that the minimum pendant dominating Estrada index of a graph G depends on the minimum pendant dominating set:

Example 3.1. *Consider the graph given in Figure 1. The possible minimum pendant dominating sets are (i) $D_1 = \{v_1, v_2, v_4\}$, (ii) $D_2 = \{v_2, v_3, v_5\}$, (iii) $D_3 = \{v_2, v_3, v_6\}$, (iv) $D_4 = \{v_2, v_3, v_4\}$, (v) $D_5 = \{v_1, v_4, v_3\}$, (vi) $D_6 = \{v_5, v_6, v_2\}$. Hence choosing D_1 as a pendant dominating set, we find*

$$A_{pe,D_1}(G) = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}.$$

Then the minimum pendant dominating spectrum containing the corresponding eigenvalues would be $\{\alpha_1(G) = 2.714,\ \alpha_2(G) = 2.141,\ \alpha_3(G) = 0.629,$

$\alpha_4(G) = -0.216$, $\alpha_5(G) = -1$, $\alpha_6(G) = -1.268\}$. Then the minimum pendant dominating Estrada index would be $EE_{pe}(G) = 26.9281968265447$.

Now, suppose we choose another pendant dominating set $D_2 = \{v_2, v_3, v_5\}$. Then similarly we would have

$$A_{pe,D_2}(G) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}.$$

Therefore the minimum pendant dominating spectrum would have the eigenvalues $\alpha_1(G) = 2.732$, $\alpha_2(G) = 2.095$, $\alpha_3(G) = 0.738$, $\alpha_4(G) = -0.477$, $\alpha_5(G) = -0.732$, $\alpha_6(G) = -1.356$. Hence the minimum pendant dominating Estrada index would be $EE_{pe}(G) = 26.9400504235982$.

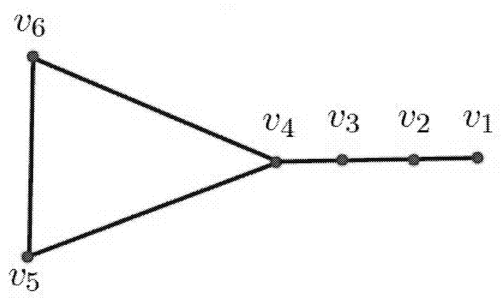

Figure 1. *The graph G in Example 1*

Now, by the eigenvalues in [31], we find formulae for the minimum pendant dominating Estrada indices of certain classical graph types including complete graph, star graph, complete bipartite graph and cocktail party graph. The proofs are straightforward and omitted:

Lemma 3.1. *For any integer $n \geqslant 2$, the minimum pendant dominating Estrada index of a complete graph K_n is equal to*

$$EE_{pe}(K_n) = e^{\frac{n-1-\sqrt{n^2-2n+9}}{2}} + e^{\frac{n-1+\sqrt{n^2-2n+9}}{2}} + (n-3)e^{-1} + n - 3.$$

Lemma 3.2. *For any integer $n \geqslant 2$, the minimum pendant dominating Estrada index of a star graph $K_{1,n-1}$ is equal to*

$$EE_{pe}(K_{1,n-1}) = e^{\sqrt{n-2}} + e^{-\sqrt{n-2}} + e^2 + n - 3.$$

Lemma 3.3. *For any integer $n \geqslant 2$, the minimum pendant dominating Estrada index of a complete bipartite graph $K_{n,n}$ is equal to*

$$EE_{pe}(K_{n,n}) = e^{\frac{n-1+\sqrt{n^2-2n+5}}{2}} + e^{\frac{n-1-\sqrt{n^2-2n+5}}{2}} + e^{\frac{-n+1+\sqrt{n^2+2n-3}}{2}} + e^{\frac{-n+1-\sqrt{n^2+2n-3}}{2}} + 2n - 4.$$

Lemma 3.4. *The minimum pendant dominating Estrada index of a cocktail party graph is equal to*

$$EE_{pe}(K_{n\times 2}) = e^{n-2+\sqrt{n^2+1}} + e^{n-2-\sqrt{n^2+1}} + (n-1)e^{-2} + e^{\frac{-1+\sqrt{5}}{2}} + e^{\frac{-1-\sqrt{5}}{2}} + (n-3)e^{-2} + e + n - 1.$$

Before showing our main results, we present a useful result:

Theorem 3.5. *(cf. [31]) Let G be a simple graph having vertex set $V = \{v_1, v_2, \cdots, v_n\}$, edge set E and let $D = \{u_1, u_2, \cdots, u_k\}$ be a minimum dominating set. If $\alpha_1, \alpha_2, \cdots, \alpha_n$ are the eigenvalues of minimum pendant dominating matrix $A_{pe}(G)$, then*

$$(i) \quad \sum_{i=1}^{n} \alpha_i = \gamma_{pe}(G),$$
$$(ii) \quad \sum_{i=1}^{n} \alpha_i^2 = 2m + \gamma_{pe}(G).$$

In the following theorem, using Theorem 1, we obtain an upper bound for the minimum pendant dominating Estrada index:

Theorem 3.6. *Let G be a graph with n vertices and m edges and let $\sum_{i=n_+ +1}^{n} \alpha_i^2 \geqslant 1$. Then*

$$EE_{pe}(G) \leqslant n - 1 + e^{\sqrt{2m+\gamma_{pe}(G)-1}}. \tag{4}$$

Proof. Let the number of positive eigenvalues of G be n_+. Since $f(x) = e^x$ monotonically increases in the interval $(-\infty, +\infty)$ and $m \neq 0$, we get

$$\begin{aligned}
EE_{pe}(G) &= \sum_{i=1}^{n} e^{\alpha_i} \\
&< n - n_+ + \sum_{i=1}^{n_+} e^{\alpha_i} \\
&= n - n_+ + \sum_{i=1}^{n_+} \sum_{k\geqslant 0} \frac{(\alpha_i)^k}{k!} \\
&= n + \sum_{k\geqslant 1} \frac{1}{k!} \sum_{i=1}^{n_+} (\alpha_i)^k \\
&\leqslant n + \sum_{k\geqslant 1} \frac{1}{k!} \Big[\sum_{i=1}^{n_+} \alpha_i^2\Big]^{\frac{k}{2}} \\
&= n + \sum_{k\geqslant 1} \frac{1}{k!} \Big[2m + \gamma_{pe}(G) - \sum_{i=n_+ +1}^{n} \alpha_i^2\Big]^{\frac{k}{2}}
\end{aligned}$$

as $\sum_{i=n_{+}+1}^{n} \alpha_i^2 \geqslant 1$. Consequently,

$$EE_{pe}(G) \leqslant n + \sum_{k\geqslant 1} \frac{1}{k!}\Big[2m + \gamma_{pe}(G) - 1\Big]^{\frac{k}{2}} = n - 1 + e^{\sqrt{2m+\gamma_{pe}(G)-1}}.$$

□

Theorem 3.7. *Let G be a graph with n vertices and m edges. Then for any integer $k_0 \geqslant 2$, we have*

$$EE_{pe}(G) \leqslant n - \gamma_{pe} - 1 - \sqrt{2m + \gamma_{pe}(G)} + \sum_{k=2}^{k_0} \frac{R_k(G) - \left(\sqrt{2m + \gamma_{pe}(G)}\right)^k}{k!} + e^{\sqrt{2m+\gamma_{pe}(G)}}.$$

Proof. Using Theorem 1 (ii) and the definition of the minimum pendant dominating Estrada index, we have

$$\begin{aligned} EE_{pe}(G) &= \sum_{k=0}^{k_0} \frac{R_k(G)}{k!} + \sum_{k\geqslant k_0+1} \frac{1}{k!}\sum_{i=1}^{n} \alpha_i^k \\ &\leqslant \sum_{k=0}^{k_0} \frac{R_k(G)}{k!} + \sum_{k\geqslant k_0+1} \frac{1}{k!}\Big(\sum_{i=1}^{n} \alpha_i^2\Big)^{\frac{k}{2}} \text{ by Inequality (3)} \\ &= \sum_{k=0}^{k_0} \frac{R_k(G)}{k!} + \sum_{k\geqslant k_0+1} \frac{\left(\sqrt{2m+\gamma_{pe}(G)}\right)^k}{k!} \\ &= \sum_{k=0}^{k_0} \frac{R_k(G)}{k!} + e^{\sqrt{2m+\gamma_{pe}(G)}} - \sum_{k=0}^{k_0} \frac{\left(\sqrt{2m+\gamma_{pe}(G)}\right)^k}{k!}. \end{aligned}$$

□

Setting $k_0 = 2$ above, we have

$$EE_{pe}(G) \leqslant n - \gamma_{pe}(G) - 1 - \sqrt{2m + \gamma_{pe}(G)} + e^{\sqrt{2m+\gamma_{pe}(G)}}.$$

4. Bounds for the minimum pendant dominating Estrada index involving the minimum pendant dominating energy of graphs

In this section, we investigate the relations between minimum pendant dominating Estrada index and the minimum pendant dominating energy. First, we state the following theorem:

Theorem 4.1. *Let G be a graph with $n \geqslant 2$ vertices and m edges. Then*

$$\alpha_1 \geq \frac{2m + \gamma_{pe}(G)}{E_{pe}(G)}. \tag{5}$$

Proof. Let a_i, b_i be two decreasing non-negative sequences with $a_i, b_i \neq 0$ and w_i be a non-negative sequence for $i = 1, 2, \ldots, n$. Then the following inequality is valid (see [11] p. 85):

$$\sum_{i=1}^{n} w_i a_i^2 \sum_{i=1}^{n} w_i b_i^2 \leqslant max \left\{ b_1 \sum_{i=1}^{n} w_i a_i, a_1 \sum_{i=1}^{n} w_i b_i \right\} \sum_{i=1}^{n} w_i a_i b_i. \tag{6}$$

For $a_i = b_i := |\alpha_i|$ and $w_i := 1$, $i = 1, 2, \ldots, n$, inequality (6) becomes

$$\sum_{i=1}^{n} |\alpha_i|^2 \sum_{i=1}^{n} |\alpha_i|^2 \leqslant max \left\{ \alpha_1 \sum_{i=1}^{n} |\alpha_i|, \alpha_1 \sum_{i=1}^{n} |\alpha_i| \right\} \sum_{i=1}^{n} |\alpha_i|^2.$$

Since

$$\sum_{i=1}^{n} |\alpha_i|^2 = \sum_{i=1}^{n} \alpha_i^2$$

and

$$\sum_{i=1}^{n} |\alpha_i| = E_{pe}(G),$$

the assertion of Theorem 4.1 directly follows from the above inequality, i.e. inequality (5) is shown. □

Theorem 4.2. *Let G be a graph with n vertices. Then*

$$EE_{pe}(G) \geqslant e^{\frac{2m+\gamma_{pe}(G)}{E_{pe}(G)}} + \frac{n-1}{e^{\frac{\frac{2m+\gamma_{pe}(G)}{E_{pe}(G)}}{n-1}}} + e^{\frac{-\gamma_{pe}(G)}{n-1}}.$$

Proof. By the definition of the minimum pendant dominating Estrada index and using arithmetic-geometric mean inequality, we obtain

$$\begin{aligned} EE_{pe}(G) &= e^{\alpha_1} + e^{\alpha_2} + \cdots + e^{\alpha_n} \\ &\geqslant e^{\alpha_1} + (n-1)\left(\prod_{i=2}^{n} e^{\alpha_i}\right)^{\frac{1}{n-1}} \\ &= e^{\alpha_1} + (n-1)e^{\frac{\sum_{i=2}^{n} e^{\alpha_i}}{n-1}} \\ &= e^{\alpha_1} + (n-1)e^{\frac{-\alpha_1}{n-1}} + e^{\frac{-\gamma_{pe}(G)}{n-1}}. \end{aligned}$$

Now we consider the following function

$$f(x) = e^x + \frac{n-1}{e^{\frac{x}{n-1}}} + e^{\frac{-\gamma_{pe}(G)}{n-1}}$$

for $x > 0$. We have

$$f(x) \geqslant e^x + \frac{n-1}{e^{\frac{x}{n-1}}} + e^{\frac{-\gamma_{pe}(G)}{n-1}}.$$

It is easy to see that f is an increasing function for $x > 0$. Hence we obtain

$$EE_{pe}(G) \geqslant e^{\frac{2m+\gamma_{pe}(G)}{E_{pe}(G)}} + \frac{n-1}{e^{\frac{\frac{2m+\gamma_{pe}(G)}{E_{pe}(G)}}{n-1}}} + e^{\frac{-\gamma_{pe}(G)}{n-1}}.$$

□

Theorem 4.3. *The minimum pendant dominating Estrada index $EE_{pe}(G)$ and the pendant dominating energy $E_{pe}(G)$ satisfy the following inequality:*

$$\frac{1}{2}E_{pe}(G)(e-1)+(n-n_+)+\gamma_{pe}\leqslant EE_{pe}(G)\leqslant n-1+e^{\frac{E_{pe}(G)}{2}}. \tag{7}$$

Proof. Lower bound: Since $e^x \geqslant 1+x$, equality holds if and only if $x=0$ and $e^x \geqslant ex$, equality holds if and only if $x=1$, we have

$$\begin{aligned}
EE_{pe}(G) &= \sum_{i=1}^{n} e^{\alpha_i} = \sum_{\alpha_i>0} e^{\alpha_i} + \sum_{\alpha_i\leqslant 0} e^{\alpha_i}\\
&\geqslant \sum_{\alpha_i>0} e\alpha_i + \sum_{\alpha_i\leqslant 0}(1+\alpha_i)\\
&= e(\alpha_1+\alpha_2+\cdots+\alpha_{n_+})+(n-n_+)+(\alpha_{n_++1}+\cdots+\alpha_n)\\
&= (e-1)(\alpha_1+\alpha_2+\cdots+\alpha_{n_+})+(n-n_+)+\sum_{i=1}^{n}\alpha_i\\
&= \frac{1}{2}E_{pe}(G)(e-1)+(n-n_+)+\gamma_{pe}.
\end{aligned}$$

Upper bound: We have

$$EE_{pe}(G)\leqslant n+\sum_{k\geqslant 1}\frac{1}{k!}\sum_{i=1}^{n_+}(\alpha_i)^k \leqslant n+\sum_{k\geqslant 1}\frac{1}{k!}\left(\sum_{i=1}^{n_+}\alpha_i\right)^k = n-1+e^{\frac{E_{pe}(G)}{2}}.$$

□

Theorem 4.4. *Let G be a graph with n vertices and m edges. Then*

$$EE_{pe}(G)-E_{pe}(G)\leqslant n-1-\sqrt{2m+\gamma_{pe}(G)}+e^{\sqrt{2m+\gamma_{pe}(G)}}.$$

Proof. By the definition of the minimum pendant dominating Estrada index, we have

$$EE_{pe}(G)=n+\sum_{i=1}^{n}\sum_{k\geqslant 1}\frac{(\alpha_i)^k}{k!}\leqslant n+\sum_{i=1}^{n}\sum_{k\geqslant 1}\frac{|\alpha_i|^k}{k!}.$$

Moreover, by considering the minimum pendant dominating energy, we get

$$EE_{pe}(G)\leqslant n+E_{pe}(G)+\sum_{i=1}^{n}\sum_{k\geqslant 2}\frac{|\alpha_i|^k}{k!}.$$

Hence

$$\begin{aligned}
EE_{pe}(G)-E_{pe}(G) &\leqslant n+\sum_{i=1}^{n}\sum_{k\geqslant 2}\frac{|\alpha_i|^k}{k!}\\
&\leqslant n-1-\sqrt{2m+\gamma_{pe}(G)}+e^{\sqrt{2m+\gamma_{pe}(G)}}.
\end{aligned}$$

□

Theorem 4.5. *Let G be a graph with n vertices and m edges. Then*

$$EE_{pe}(G)+E_{pe}(G)\leqslant n-1-\gamma_{pe}+e^{E_{pe}(G)}.$$

Proof. By the definition of the minimum pendant dominating Estrada index, we have

$$\begin{aligned}
EE_{pe}(G) = \sum_{i=1}^{n} e^{\alpha_i} = \sum_{i=1}^{n}\sum_{k\geqslant 0}\frac{(\alpha_i)^k}{k!} &= n-\gamma_{pe}(G)+\sum_{i=1}^{n}\sum_{k\geqslant 2}\frac{\alpha_i^k}{k!}\\
&< n-\gamma_{pe}(G)+\sum_{i=1}^{n}\sum_{k\geqslant 2}\frac{|\alpha_i|^k}{k!}\\
&= n-\gamma_{pe}(G)+\sum_{k\geqslant 2}\frac{1}{k!}\sum_{i=1}^{n}|\alpha_i|^k\\
&\leqslant n-\gamma_{pe}(G)+\sum_{k\geqslant 2}\frac{1}{k!}\left(\sum_{i=1}^{n}|\alpha_i|\right)^k\\
&= n-1-\gamma_{pe}(G)-E_{pe}(G)+\sum_{i=1}^{n}\sum_{k\geqslant 0}\frac{(E_{pe}(G))^k}{k!}.
\end{aligned}$$

□

Theorem 4.6. *Let G be a graph with n vertices. Then*

$$EE_{pe}(G) \leqslant n-1+e^{E_{pe}(G)}.$$

Proof. By the definition of the minimum pendant dominating Estrada index, we have

$$\begin{aligned}
EE_{pe}(G) &\leqslant n+\sum_{i=1}^{n}\sum_{k\geqslant 1}\frac{|\alpha_i|^k}{k!}\\
&\leqslant n+\sum_{k\geqslant 1}\frac{1}{k!}\left(\sum_{i=1}^{n}|\alpha_i|^k\right)\\
&= n+\sum_{k\geqslant 1}\frac{(E_{pe}(G))^k}{k!}
\end{aligned}$$

which implies

$$EE_{pe}(G) \leqslant n-1+e^{E_{pe}(G)}.$$

□

Concluding Remarks

In this paper, the minimum pendant dominating Estrada index of a graph is introduced. We also obtained some bounds for this new index. Finally, we investigate the relations between the new Estrada index and the new energy. It is possible to apply the ideas obtained and proved here can be applied to specific graph classes, to derived graphs and to graph operations. Also these methods can be applied to molecular graphs to get some physico-chemical properties of the molecules under investigation.

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