Journal of Computer and Mathematical Sciences, *Vol.10(3),565-573 March 2019* *ISSN 0976-5727 (Print)*
(An International Research Journal), *www.compmath-journal.org* *ISSN 2319-8133 (Online)*

Bounds for the Eigen Values and Energy of Degree Product Adjacency Matrix of A Graph

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(Received on: March 14, 2019)

ABSTRACT

In this article, we obtain a bound for eigen values of degree product adjacency matrix [$DPA(G)$] and also obtain some lower bounds for the degree product adjacency energy of graph G.

Mathematical Subject Classification:05C07, 05C50.

Keywords: Energy, Degree product adjacency energy.

1. INTRODUCTION

Let G be a simple, connected and finite graph with order n and size m. d_i is the degree of the vertex v_i, where d_i is the number of edges incident to the vertex v_i. For undefined terminologies we refer[7]. A molecular graph is a graph in which the vertices corresponds to the atoms and edges corresponds to the bonds. Chemical graph theory is a branch of mathematical chemistry which has an imporatant effect on the development of the chemical sciences.

The adjacency matrix $A(G)$ of a graph G will be (0, 1) matrix and is defined as

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

If $\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_n$ are the eigen values of $A(G)$. Then the energy of a graph G is defined as the sum of absolute values of the eigen values of adjacent matrix of graph G. This concept was introduced by I. Gutman in[5].

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

The above defined energy explained is the way of pure mathematical concept. But when a molecular graph is used to model a π-electron system, the energy of the graph has been shown to be a good approximation of the binding energy of the π-electrons. Motivation of the above defined energy has been well explained in[6]. The total molecular orbital energy of all π-electrons in a molecule, by Hückel molecule orbit model is given by

$$E_\pi = n_e\alpha + \beta\sum_{i=1}^{n}\eta_i\lambda_i$$

Where $n_e\alpha$ corresponds to the energy of n_e isolated p-electron, β is a constant, η_i is the number of π-electrons in the i^{th} molecular orbital and λ_i's are the eigen values of the corresponding molecular graph. Since the author in[5] was interested only in the binding energy of the π-electrons, so he considered the non-trivial part of the above equation i.e., $E = \sum_{i=1}^{n}\eta_i\lambda_i$. For most conjugated π-electron systems of chemical interests, all bonding molecular orbitals are doubly occupied and antibonding molecular orbitals are unoccupied. This leads to the fact that

$$\eta_i = \begin{cases} 2, & \text{if } \lambda_i > 0, \\ 0, & \text{if } \lambda_i < 0. \end{cases}$$

Hence $E = 2\sum_{\lambda_i > 0}\lambda_i$. Notice that for a simple graph $\sum_{i=n}^{n}\lambda_i = trace(A(G)) = 0$ then $E = \sum_{i=1}^{n}|\lambda_i|$.

The Cauchy-Schwarz inequality[2] states that if $(a_1, a_2, a_3, \ldots, a_n)$ and $(b_1, b_2, b_3, \ldots, b_n)$ are real n-vectors then,

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \le \left(\sum_{i=1}^{n} a_i^{\,2}\right)\cdot\left(\sum_{i=1}^{n} b_i^{\,2}\right)$$

Motivated by the work of C. Adiga *et al.*[1] and H. S. Ramane *et al.*[11], we introduce the concept of degree product adjacency energy[8], which is defined as follows.

Definition

Let G be a simple, connected graph with n-vertices $v_1, v_2, v_3, \ldots, v_n$ and d_i be the degree of the vertex v_i, $\forall i = 1, 2, \ldots, n$. Then the degree product adjacency matrix $[DPA(G)]$ of a graph G is $[d_{ij}]$ i.e.,

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

The degree product adjacency matrix $[DPA(G)]$ is a real symmetric matrix and its eigen values are $\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_n$. The order of eigen values be arranged as $\alpha_1 \ge \alpha_2 \ge \alpha_3 \ge \ldots \ge \alpha_n$. In the similar way of adjacency energy, the degree product adjacency energy of a graph defined and is denoted by as follows,

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

In this article, we establish the results on bound for the largest eigen value of *DPA*(*G*) and also obtain the lower bounds for the degree product adjacency energy of a graph *G*.

2. RESULTS

To present the complete results, some important theorems which are used throught out the paper are mentioned below.

Theorem 2.1.[10] Suppose a_i and b_i, $1 \le i \le n$ are positive real numbers, then

$$\sum_{i=1}^{n} a_i^{\,2} \sum_{i=1}^{n} b_i^{\,2} \le \frac{1}{4}\left(\sqrt{\frac{M_1 M_2}{m_1 m_2}} + \sqrt{\frac{m_1 m_2}{M_1 M_2}}\right)^2 \left(\sum_{i=1}^{n} a_i b_i\right)^2$$

Where $M_1 = \max_{1 \le i \le n}(a_i); M_2 = \max_{1 \le i \le n}(b_i); m_1 = \min_{1 \le i \le n}(a_i); m_2 = \min_{1 \le i \le n}(b_i)$

Theorem 2.2.[9] Let a_i and b_i, $1 \le i \le n$ are nonnegative real numbers, then

$$\sum_{i=1}^{n} a_i^{\,2} \sum_{i=1}^{n} b_i^{\,2} - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \le \frac{n^2}{4}\left(M_1 M_2 - m_1 m_2\right)^2$$

where $M_1 M_2$ and $m_1 m_2$ are defined similarly to Theorem 2.1.

Theorem 2.3.[3] Suppose a_i and b_i, $1 \le i \le n$ are positive real numbers, then

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \le \mu(n)(A-a)(B-b)$$

where a, b, A and B are real constants, that for each i, $1 \le i \le n$, $a \le a_i \le A$ and $b \le b_i \le B$ Further,

$$\mu(n) = n\left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor\right).$$

Theorem 2.4.[4] Let a_i and b_i, $1 \le i \le n$ are nonnegative real numbers, then

$$\sum_{i=1}^{n} b_i^{\,2} + rR\sum_{i=1}^{n} a_i^{\,2} \le (r+R)\left(\sum_{i=1}^{n} a_i b_i\right)$$

where r and R are real constants. So that for each i, $1 \le i \le n$ holds $ra_i \le b_i \le Ra_i$

2.1 Bounds for the largest eigen value of *DPA*(*G*)

We need the following Lemma to prove the further results.

Lemma A. If the trace $[DPA(G)] = 0$, then the eigen values obtained from $DPA(G)$ matrix satisfies the following,

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

(ii) $\sum_{i=1}^{n} \alpha_i^2 = trace(DPA(G))^2$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij} d_{ji}, \forall i \sim j$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} (d_{ij})^2$$

$$= 2 \sum_{1 \le i < j \le n} (d_i \times d_j)^2$$

$$= 2P$$

Where $P = \sum_{1 \le i < j \le n} (d_i \times d_j)^2$

Theorem 2.5. If G be a graph with n-vertices, then

$$\alpha_1 \le \sqrt{\frac{2P(n-1)}{n}}$$

Proof. Consider the graph G with n-vertices. Let $DPA(G)$ be the degree product adjacency matrix of graph G and $\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_n$ are the eigen values obtained from the $DPA(G)$ matrix, where α_1 is the largest eigen value and the bound for α_1 is calculated by using cauchy-schwarz inequality i.e.,

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \le \left(\sum_{i=1}^{n} a_i^2\right).\left(\sum_{i=1}^{n} b_i^2\right)$$

Let $a_i = 1$ and $b_i = \alpha_i$, $\forall i = 2, 3, \ldots, n$ then the inequality becomes,

$$\left(\sum_{i=1}^{n} (1)(\alpha_i)\right)^2 \le \left(\sum_{i=1}^{n} 1^2\right).\left(\sum_{i=1}^{n} \alpha_i^2\right) \tag{1}$$

From Lemma A(i),

$$\sum_{i=1}^{n} \alpha_i = 0$$

$$\alpha_1 + \sum_{i=2}^{n} \alpha_i = 0 \tag{2}$$

$$\left(\sum_{i=2}^{n} \alpha_i\right)^2 = (-\alpha_1)^2$$

And from Lemma A(ii)

$$\sum_{i=1}^{n}(\alpha_i)^2 = 2P$$

$$(\alpha_1)^2 + \sum_{i=2}^{n}(\alpha_i)^2 = 2P$$

$$\sum_{i=2}^{n}(\alpha_i)^2 = 2P - (\alpha_1)^2 \qquad (3)$$

Substituting (2) and (3) in (1), we get

$$(-\alpha_i)^2 \le (n-1)(2P - \alpha_i^{\ 2})$$

$$\alpha_1^{\ 2} \le 2P(n-1) - \alpha_i^{\ 2}(n-1)$$

$$\alpha_1 \le \sqrt{\frac{2P(n-1)}{n}}$$

The equality relation for α_1 holds for the regular graphs, P_2 and W_4.

Theorem 2.6. If G be a graph with n-vertices, then
$\sqrt{2P} \le E_{DPA}(G) \le \sqrt{2nP}$

Proof. Consider a graph G with n-vertices. Let $DPA(G)$ be the degree product adjacency matrix of a graph G and $\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_n$ are the eigen values of the matrix $DPA(G)$. Now we consider the cauchy-schwarz inequality to prove the theorem,

- **Proof for Right hand side bond:**

Let us assume that $a_i = 1$ and $b_i = |\alpha_i|$, $\forall i = 1, 2, \ldots, n$.

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \le \left(\sum_{i=1}^{n} a_i^{\ 2}\right).\left(\sum_{i=1}^{n} b_i^{\ 2}\right)$$

$$\left(\sum_{i=1}^{n}(1)\,|\,\alpha_i\,|\right)^2 \le \left(\sum_{i=1}^{n}(1)^2\right).\left(\sum_{i=1}^{n}|\,\alpha_i\,|^2\right)$$

$$\left(\sum_{i=1}^{n}|\,\alpha_i\,|\right)^2 \le n\left(\sum_{i=1}^{n}|\,\alpha_i\,|^2\right)$$

After simplification by using the Lemma A.

$$E_{DPA}(G) \le \sqrt{2nP} \qquad (4)$$

- **Proof for Left hand side bond:**

We know that,

$$\left(\sum_{i=1}^{n} |\alpha_i|\right)^2 \geq \sum_{i=1}^{n} |\alpha_i|^2$$

By using the Lemma A, we conclude that

$$E_{DPA}(G) \geq \sqrt{2P} \qquad (5)$$

From equation (4) and (5),

$$\sqrt{2P} \leq E_{DPA}(G) \leq \sqrt{2nP}$$

2.2 Lower bounds for the degree product adjacency energy [$E_{DPA}(G)$]

Theorem 2.7. Let G be a graph with n-vertices and m-edges. Suppose $|\alpha_1| \geq |\alpha_2| \geq |\alpha_3| \geq \ldots \geq |\alpha_n|$ are the eigen values of $DPA(G)$, then the following inequality holds.

$$E_{DPA}(G) \geq \frac{2\sqrt{2nP|\alpha_1||\alpha_n|}}{|\alpha_1| + |\alpha_n|}$$

Proof. Consider a graph G with n-vertices and $|\alpha_1| \geq |\alpha_2| \geq |\alpha_3| \geq \ldots \geq |\alpha_n|$ are the eigen values of $DPA(G)$, where $|\alpha_1|$ and $|\alpha_n|$ are the maximum and minimum eigen values of $|\alpha_i|$'s respectively.

We have the inequality by the theorem 2.1,

$$\sum_{i=1}^{n} a_i^{\,2} \sum_{i=1}^{n} b_i^{\,2} \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^{n} a_i b_i\right)^2$$

Assume $a_i = 1$, $b_i = |\alpha_i|$, $M_1M_2 = |\alpha_1|$ and $m_1m_2 = |\alpha_n|$ then,

$$\sum_{i=1}^{n} 1^2 \sum_{i=1}^{n} |\alpha_i|^2 \leq \frac{1}{4}\left(\sqrt{\frac{|\alpha_1|}{|\alpha_n|}} + \sqrt{\frac{|\alpha_n|}{|\alpha_1|}}\right)^2 \left(\sum_{i=1}^{n} (1)|\alpha_i|\right)^2$$

From Lemma A,

$$n2P \leq \frac{1}{4}\left[\frac{(|\alpha_1| + |\alpha_n|)^2}{|\alpha_1||\alpha_n|}\right](E_{DPA}(G))^2$$

$$(E_{DPA}(G))^2 \geq \frac{8nP|\alpha_1||\alpha_n|}{(|\alpha_1| + |\alpha_n|)^2}$$

$$E_{DPA}(G) \geq \frac{2\sqrt{2nP|\alpha_1||\alpha_n|}}{|\alpha_1| + |\alpha_n|}$$

Theorem 2.8. Let G be a graph with n-vertices, then the following inequality holds.

$$E_{DPA}(G) \geq \sqrt{2nP - \frac{n^2}{4}\left(|\alpha_1| - |\alpha_n|\right)^2}$$

Proof. Consider a graph G with order n and size m. Let $|\alpha_1| \geq |\alpha_2| \geq |\alpha_3| \geq \ldots \geq |\alpha_n|$ be the eigen values of $DPA(G)$ matrix, where $|\alpha_1|$ and $|\alpha_n|$ are the maximum and minimum eigen values respectively.

From Theorem 2.2 we have the inequality,

$$\sum_{i=1}^{n} a_i^{\,2} \sum_{i=1}^{n} b_i^{\,2} - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \frac{n^2}{4}\left(M_1 M_2 - m_1 m_2\right)^2$$

Assume $a_i = 1$, $b_i = |\alpha_i|$, $M_1M_2 = |\alpha_1|$ and $m_1m_2 = |\alpha_n|$ in the above inequality,

$$\sum_{i=1}^{n} 1^2 \sum_{i=1}^{n} |\alpha_i|^2 - \left(\sum_{i=1}^{n} (1)|\alpha_i|\right)^2 \leq \frac{n^2}{4}\left(|\alpha_1| - |\alpha_n|\right)^2$$

From Lemma A,

$$n2P - (E_{DPA}(G))^2 \leq \frac{n^2}{4}\left(|\alpha_1| - |\alpha_n|\right)^2$$

$$E_{DPA}(G) \geq \sqrt{2nP - \frac{n^2}{4}\left(|\alpha_1| - |\alpha_n|\right)^2}$$

Theorem 2.9. Let G be a graph with n-vertices, then the following inequality holds.

$$E_{DPA}(G) \geq \sqrt{2nP - \mu(n)\left(|\alpha_1| - |\alpha_n|\right)^2}$$

Proof. Consider a graph G with order n and size m. Let $|\alpha_1| \geq |\alpha_2| \geq |\alpha_3| \geq \ldots \geq |\alpha_n|$ be the eigen values of $DPA(G)$ matrix, where $|\alpha_1|$ and $|\alpha_n|$ are the maximum and minimum eigen values respectively.

Consider inequality from the Theorem 2.3,

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \mu(n)(A-a)(B-b)$$

Now assume that $a_i = b_i = |\alpha_i|$, $A = B = |\alpha_1|$ and $a = b = |\alpha_n|$, then the inequality reduces to

$$\left| n\sum_{i=1}^{n} |\alpha_i|^2 - \left(\sum_{i=1}^{n} |\alpha_i|\right)^2 \right| \leq \mu(n)(|\alpha_1| - |\alpha_n|)(|\alpha_1| - |\alpha_n|)$$

From Lemma A,

$$\left| 2nP - \left(E_{DPA}(G)\right)^2 \right| \leq \mu(n)(|\alpha_1| - |\alpha_n|)^2$$

$$E_{DPA}(G) \geq \sqrt{2nP - \mu(n)(|\alpha_1| - |\alpha_n|)^2}$$

Theorem 2.10. Let G be a graph with n-vertices, then the following inequality holds.

$$E_{DPA}(G) \geq \frac{2P + n|\alpha_1||\alpha_n|}{|\alpha_1| + |\alpha_n|}$$

Proof. Consider a graph G with order n and size m. Let $|\alpha_1| \geq |\alpha_2| \geq |\alpha_3| \geq \ldots \geq |\alpha_n|$ be the eigen values of $DPA(G)$ matrix, arranged in non-increasing order, where $|\alpha_1|$ and $|\alpha_n|$ are the maximum and minimum eigen values respectively.

We make use of the inequality from the Theorem 2.4,

$$\sum_{i=1}^{n} b_i^{\,2} + rR\sum_{i=1}^{n} a_i^{\,2} \leq (r+R)\left(\sum_{i=1}^{n} a_i b_i\right)$$

Assume $b_i = |\alpha_i|$, $a_i = 1$, $r = |\alpha_n|$ and $R = |\alpha_1|$, then the inequality implies to

$$\sum_{i=1}^{n} |\alpha_i|^2 + |\alpha_n||\alpha_1|\sum_{i=1}^{n} 1^2 \leq (|\alpha_n| + |\alpha_1|)\left(\sum_{i=1}^{n} (1)|\alpha_i|\right)$$

From Lemma A,

$$2P + (|\alpha_n||\alpha_1|)(n) \leq (|\alpha_n| + |\alpha_1|)E_{DPA}(G)$$

$$E_{DPA}(G) \geq \frac{2P + |\alpha_n||\alpha_1|(n)}{|\alpha_n| + |\alpha_1|}$$

ACKNOWLEDGEMENT

The authors are thankful to university Grants Commission (UGC), Govt. of India for financial support through research grant under F1-17.1/2017-18/RGNF-2017-18-SC-KAR-39176 /(SA-III/Website).

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