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Calculation of Maximum Degree Energy Using Integrals

K. Saravanan[1], K.Srinivasa Rao[2]
[1]*Research Scholar, Department of Mathematics Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya, Kanchipuram, Tamilnadu*

***Abstract*—In this paper, maximum degree energy is computed by means of a certain integral involving the characteristic polynomial and the with help of this integral we obtain $E_M(S_n^4) < E_M(S_n^3), \ \forall n \geq 5$**

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1. INTRODUCTION

The graph energy is one of the most important graph invariants in chemical graph theory. It was originally inspired [1] by the Hückel molecular orbital approximation, where it relates to the π- electron energy. The energy E(G) of a graph G is defined to be the sum of the absolute values of its eigenvalues. Hence if A(G) is the adjacency review articles matrix of G and if $\lambda_1, \lambda_2, \ldots, \lambda_n$re its eigenvalues, then. $E(G) = \sum_{i=1}^{n} |\lambda_i|$ Numerous review articles have been written on the energy of graphs, see e.g. [1]-[11].

One of the ways of studying graphs is to make use of matrices. Several graph matrices have been defined and used in literature. Apart from the adjacency matrix, the incidency and Laplacian matrices are the most important ones. Another matrix, the maximum degree matrix was defined by Adiga and Smitha in [12]. Let G be a simple graph with n vertices $v_1, v_1, \ldots, v_n$ and let d_i be the degree of v_i for $i = 1, 2, \cdots, n$. Define

$$d_{ij} = \begin{cases} \max\{d_i, d_j\} & if\ v_i\ and\ v_j are\ adjacent \\ 0 & othereise \end{cases}$$

Then the n × n matrix M (G) =(d_{ij}) is called the maximum degree matrix of G, [12]. Let $\mu_1, \mu_2, \cdots, \mu_n$ be the maximum degree eigenvalues of M (G). Since M (G) is a real symmetric matrix with zero trace, these maximum degree eigenvalues are real with sum equal to zero. That is, $\sum_{i=0}^{n} \mu_i = 0$

The maximum degree energy of a graph G is defined as $E_M(G) = \sum_{i=0}^{n} |\mu_i|$

It is shown that if the maximum degree energy of a graph is rational, then it must be an even integer, [12].

2. MAXIMUM DEGREE ENERGY

In this section, maximum degree energy is computed by means of a certain integral involving the characteristic polynomial and obtain $E_M(S_n^4) < E_M(S_n^3), \ \forall n \geq 5$

Lemma 2.1. *For every real number a, we have* $\int_0^\infty \frac{1}{x^2} \ln(1 + a^2x^2)\, dx, \ \forall n \geq 5$

Theorem 2.1. *Let* $\phi(x) = \det(xI - M(G))$ *be the characteristic polynomial of the maximum degree matrix of a graph G with n vertices. Then maximum degree energy* E_M *(G) of given by the following integral:*

$$E_M(G) = \frac{1}{\pi} \int_0^\infty \frac{1}{x^2} \ln\left(x^{2n} \phi\left(\frac{i}{x}\right) \phi\left(-\frac{i}{x}\right) \right) dx \quad = \frac{2}{\pi} \int_0^\infty n \ln x + \ln|(\phi(i/x))|\, dx$$

Proof. we can write the characteristic polynomial as $\phi(x) = \prod_{j=1}^{n} (x - \mu_j)$

Where $\mu_1, \mu_2, \cdots, \mu_n$ are the maximum degree eigenvalues. Now note that

$$\phi(i/x)\phi(-i/x) = \prod_{j=1}^{n} \left(i/x - \mu_j \right)\left(-\ i/x - \mu_j \right) = \prod_{j=1}^{n} (\frac{1}{x^2} + \mu_j^2)$$

So $x^{2n}\, \phi(i/x)\phi(-i/x) = \prod_{j=1}^{n} (1 + \mu_j^2 x^2)$

and consequently

$$\int_0^\infty \frac{1}{x^2}\ln\left(x^{2n}\phi(i/x)\phi(-i/x)\right)dx = \sum_{j=0}^{n}\int_0^\infty \frac{1}{x^2}\ln\left(1+\mu_j^2x^2\right)$$

By lemma 1.1 it follows that

$$\int_0^\infty \frac{1}{x^2}\ln\left(x^{2n}\phi(i/x)\phi(-i/x)\right)dx = \sum_{j=0}^{n}\pi\left|\mu_j\right| = \pi E_M(G)$$

and the first identity follows. Since $\phi(x)$ is a polynomial with real coefficients, we have $\phi(i/x) = \phi(-i/x)$ for real values of *x*. Thus

$$\phi(i/x)\phi(-i/x) = |\,\phi(i/x)|^2$$

and we obtain

$$E_M(G) = \frac{1}{\pi}\int_0^\infty \frac{1}{x^2}\ln(x^{2n}|\,\phi(i/x)|^2)\,dx$$

$$E_M(G) = \frac{2}{\pi}\int_0^\infty (n\ln x + ln\,|\phi(i/x)|)dx$$

Theorem 2.2. [12] If G is bipartite and μ is an eigenvalue of G with respect to maximum degree matrix with multiplicity m, then −μ is also an eigenvalue with multiplicity m

Lemma 2.2. Let G be a bipartite graph with n vertices. If $m \not\equiv n \bmod 2$, the the coefficient of x^m in the characteristic polynomial of G with respect to maximum degree matrix is 0

Proof. If G is bipartite graph, then from Theorem 2.2 the spectrum of maximum degree matrix is symmetric with respect to 0. Hence the required result.

Theorem 2.3. Let the characteristic polynomial of maximum degree matrix of a graph G be $\phi(x) = \det\left(xI - M(g)\right) = \sum_{k=0}^{n} a_k x^n$

The maximum degree energy of G can be expressed as

$$E_M(G) = \frac{1}{\pi}\int_0^\infty \frac{1}{x^2}ln\left[\left(\sum_{j\le n/2}(-1)^j a_{2j}x^{2j}\right)^2 + \left(\sum_{j\le (n-1)/2}(-1)^j a_{2j+1}x^{2j+1}\right)^2\right]dx$$

In particular, if G is bipartite graph, then

$$E_M(G) = \frac{2}{\pi}\int_0^\infty \frac{1}{x^2}ln\left(\sum_{j\le n/2}(-1)^j a_{2j}x^{2j}\right)dx$$

Proof. We note that

$$x^{2n}\phi(i/x) = \sum_{k=0}^{n} a_k i^{n-k}x^k \;\; = i^n\left(\sum_{j\le n/2}(-1)^j a_{2j}x^{2j} - i\sum_{j\le (n-1)/2}(-1)^j a_{2j+1}x^{2j+1}\right)$$

and analogously

$$x^{2n}\phi(-\,i/x) = \sum_{k=0}^{n} a_k(-i)^{n-k}x^k \;\; = (-i)^n\left(\sum_{j\le n/2}(-1)^j a_{2j}x^{2j} + i\sum_{j\le (n-1)/2}(-1)^j a_{2j+1}x^{2j+1}\right)$$

It follows that

$$x^{2n}\phi(i/x)\phi(-\,i/x) = \left(\sum_{j\le n/2}(-1)^j a_{2j}x^{2j}\right)^2 + \left(\sum_{j\le (n-1)/2}(-1)^j a_{2j+1}x^{2j+1}\right)^2$$

Hence the required result is a direct consequence of Theorem 1.1

If G is a bipartite graph, then from Lemma 2.2, we have $a_{2j+1} = 0$, for all *j*. Hence

$$E_M(G) = \frac{2}{\pi}\int_0^{\infty} \frac{1}{x^2} ln\left(\sum_{j\le n/2} (-1)^j a_{2j} x^{2j}\right) dx$$

Definition.
The graph S_n^3 obtained by attaching $n-3$ pendent vertices to one of the vertices of the cycle C_3.

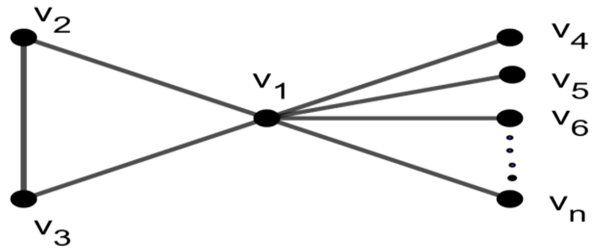

Figure 1. S_n^3 graph

Lemma 2.3. Let $n \geq 4$ then the characteristic polynomial of S_n^3 is

$$\mu^{n-4}(\mu+2)(\mu^3 - 2\mu^2 - (n-1)^3\mu + 2(n-3)(n-1)^2$$

Proof. The maximum degree matrix of S_n^3 according to the vertex labeling shown in Fig.1 is of order $n \times n$ and is given by

$$M(S_n^3) = \begin{pmatrix} A_{3\times 3} & B_{3\times(n-3)} \\ B^T_{(n-3)\times 3} & O_{(n-3)\times(n-3)} \end{pmatrix}$$

Where $A = \begin{pmatrix} 0 & n-1 & n-1 \\ n-1 & 0 & 2 \\ n-1 & 2 & 0 \end{pmatrix}$, $B = \begin{pmatrix} n-1 & n-1 & \cdots & n-1 \\ 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \end{pmatrix}$ and O is the null matrix of size $(n-3) \times (n-3)$.

If R_i is the i^{th} row of the determinant $|\mu I - M(S_n^3)|$, then $R_2 = n-1, -\mu, 2, 0, \ldots, 0)$ and $R_3 = n-1, 2, -\mu, 0, \ldots, 0)$. Replacing R_2 by $R_2 - R_3$, we get the second row as $(\mu+2)(0, -1, 1, 0, \ldots, 0)$. Hence $(\mu+2)$ is one of the factors of $|\mu I - M(S_n^3)|$ Replacing R_i by $R_i - R_j$ for *j = 4, 5, …, n-1*, we conclude that μ is the common factor at each row between 4th and (n-1)-th. Hence μ^{n-4} is one of the factors of $|\mu I - M(S_n^3)|$. Using elementary mathematical simplifications, we get the rest of the result.

Definition.
The graph S_n^4 obtained by attaching $n-4$ pendent vertices to one of the vertices of the cycle C_4.

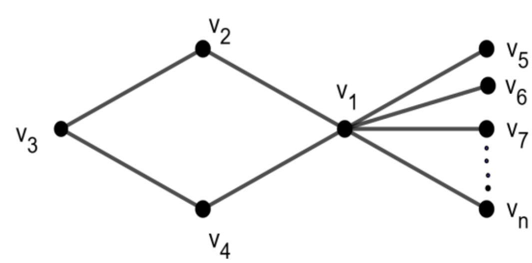

Figure 2. S_n^4 graph

Lemma 2.4. Let $n \geq 5$ then the characteristic polynomial of S_n^4 is

$$\mu^{n-4}(\mu^4 - n((n-2)(n-4)+4)\mu^2 + 8(n-4)(n-2)^2)$$

Proof. The maximum degree matrix of S_n^4 according to the vertex labeling shown in fig.1 is of size $n \times n$ and given by

$$M(S_n^3) = \begin{pmatrix} A_{4\times 4} & B_{4\times(n-4)} \\ B^T_{(n-4)\times 4} & O_{(n-4)\times(n-3)} \end{pmatrix}$$

Where $A=\begin{pmatrix} 0 & n-2 & 0 & n-2 \\ n-2 & 0 & 2 & 0 \\ 0 & 2 & 0 & 2 \\ n-2 & 0 & 2 & 0 \end{pmatrix}$, $B=\begin{pmatrix} n-2 & n-2 & ... & n-2 \\ 0 & 0 & ... & 0 \\ 0 & 0 & ... & 0 \\ 0 & 0 & ... & 0 \end{pmatrix}$ and O is the null matrix of size $(n-4)\times(n-4)$

Let R_i is the i^{th} row of the determinant $|\mu I - M(S_n^4)|$. Replacing R_i by $R_i - R_{i+1}$ for $i = 5,6, ..., n-1$, we conclude that μ is the common factor at each row between 5th and (n-1)-th.. Also replacing $C_n - C_{n-1}$. we get μ is the common factor. Hence μ^{n-4} is one of the factors of $|\mu I - M(S_n^4)|$. Using elementary mathematical simplifications, we get the rest of the result.

Theorem 2.4. *Let G be a unicyclic graph with* $n \geq 5$ *vertices. Then*

$$E_M(S_n^4) < E_M(S_n^5)$$

Proof. We have from Lemma 2.3.

$$|\mu I - M(S_n^3)| = \mu^{n-4}\left[\mu^4 - \left((n-1)^3+4\right)\mu^2 - 4(n-1)\mu + 4(n-3)(n-1)^2\right]$$

Also from Lemma 2.4, we have

$$|\mu I - M(S_n^4)| = \mu^{n-4}\left[\mu^4 - n\left((n-2)(n-4)+4\right)\mu^2 + 8(n-4)(n-2)^2\right]$$

By theorem 2.3, we have

$$E_M(S_n^4) - E_M(S_n^3) = \frac{1}{\pi}\int_0^\infty \frac{1}{x^2}\left[\frac{(1+n\left((n-2)(n-4)+4\right)x^2+8(n-4)(n-2)^2x^4)^2}{(1+((n-1)^3+4)x^2+4(n-3)(n-1)^2x^4)^2+(4(n-1)x^3)^2}\right]dx$$

Let

$$f(x) = \left[1+n\left((n-2)(n-4)+4\right)x^2+8(n-4)(n-2)^2x^4\right]^2$$
$$-[1+((n-1)^3+4)x^2+4(n-3)(n-1)^2x^4]^2 - 16(n-1)^2x^6$$

Then

$$f(x) = 2(n(n-2)(n-4)-(n-1)(n+1)(n-3))x^2$$
$$+[n^2(n-2)(n-4)\left((n-2)(n-4)+8\right)+16(n^2-1)+16(n-2)^2(n-4)$$
$$-8(n-1)^2(n-3)-8(n-1)^2-(n-1)^6]x^4$$
$$+[16n(n-2)^2(n-4)\left((n-2)(n-4)^2+4\right)-8(n-1)^2((n-3)((n-1)^3+4)-16(n-1)^2]x^6$$
$$+[64(n-2)^4(n-4)^2-16(n-1)^4(n-3)^2]x^8$$

It is clear that $f(x) < 0, \ \forall n \geq 5$

Hence $E_M(S_n^4) < E_M(S_n^5)$

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