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ON NEW BOUNDS FOR ENERGY OF GRAPHS

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ABSTRACT. The term energy was first coined by I. Gutman in chemistry, while finding the total $\pi-$electron energy of conjugated carbon compounds. In 1971 McClelland obtained both lower and upper bounds for $\pi-$electron energy. In this paper we established new bounds for energy of graphs and it also contains bounds for the largest eigenvalue and the absolute smallest eigenvalue.

1. INTRODUCTION

Let $G=(V,E)$ be a simple, connected and undirected graph with n vertices and m edges. Given a graph G, the energy of G with n vertices is defined by $\mathcal{E}(G)=\sum_{i=1}^{n}|\lambda_i|$, where $\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_n$ are eigenvalues of G which are obtained from its adjacency matrix. The studies on graph energy can be seen in papers [4–6]. For detailed survey on applications on graph energy, see papers [1–3].

McClelland gave bounds [9] for energy of graph which is true for any graph

$$\sqrt{2m+n(n-1)|det(A)|^{\frac{2}{n}}}\leq\mathcal{E}(G)\leq\sqrt{2mn}.$$

Koolen and Moulton obtained upper bounds [7] for graph energy in terms of m and n as

$$\mathcal{E}(G)\leq\left(\frac{2m}{n}\right)+\sqrt{(n-1)\Big(2m-\left(\frac{2m}{n}\right)^2\Big)}\ \text{ for } 2m\geq n.$$

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and obtained an upper bound for bipartite graph [8] as

$$\mathcal{E}(G) \leq 2\Big(\frac{2m}{n}\Big) + \sqrt{(n-2)\Big(2m - 2\Big(\frac{2m}{n}\Big)^2\Big)} \text{ for } 2m \geq n.$$

Also they proved that for a graph G with n vertices $\mathcal{E}(G) \leq \frac{n}{2}(1+\sqrt{n})$.

We begin with proving the following lemmas by making use of the elementary results on eigenvalues of graphs.

If $\lambda_1, \lambda_2, \cdots, \lambda_n$ are eigenvalues of graph G with m vertices and n edges then

1. $\sum_{i=1}^{n} \lambda_i = 0$ and $\sum_{i=1}^{n} \lambda_i^2 = 2m = \sum_{i=1}^{n} |\lambda_i|^2$. Further $\prod_{i=1}^{n} \lambda_i = det(A)$.
2. $\sum_{i=1}^{n} |\lambda_i|^2 = 2m \Rightarrow |\lambda_i|^2 \leq 2m \Rightarrow |\lambda_i| \leq \sqrt{2m}$.
3. $|\lambda_i|^2 \leq \sqrt{2m}|\lambda_i| \ \forall i$ and $|\lambda_i||\lambda_j| \leq \sqrt{2m}|\lambda_j| \ \forall i \neq j$.
4. For all connected graphs G the largest eigenvalue satisfies $\lambda_1 \geq \frac{2m}{n} \geq 1$.
5. $|det(A)| \leq (2m)^{\frac{n}{2}}$.

2. Main result

Lemma 2.1. *Let λ_1 be the largest eigenvalue of graph G with n vertices and m edges then*

$$\begin{aligned} \lambda_1 \leq \sqrt{m} \quad &\textit{if} \quad \lambda_1 \leq \sqrt{2m-\lambda_1^2}. \\ \lambda_1 \geq \sqrt{m} \quad &\textit{if} \quad \lambda_1 \geq \sqrt{2m-\lambda_1^2}. \end{aligned}$$

Proof. If $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of the graph G then $\lambda_1 + \lambda_2 + \cdots + \lambda_n = 0$ which implies $\lambda_2 + \cdots + \lambda_n = -\lambda_1$. Since λ_1 is positive, $\lambda_2 + \cdots + \lambda_n$ is negative quantity. But $\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2 = 2m$.

Also, $\lambda_2 + \lambda_3 + \cdots + \lambda_n \leq \sqrt{\lambda_2^2 + \lambda_3^2 + \cdots + \lambda_n^2}$ if $\lambda_2 + \lambda_3 + \cdots + \lambda_n$ is negative quantity; $\sqrt{\lambda_2^2 + \lambda_3^2 + \cdots + \lambda_n^2} \leq \lambda_2 + \lambda_3 \cdots + \lambda_n$ if $\lambda_2 + \lambda_3 + \cdots + \lambda_n$ is positive quantity; i.e, $-\lambda_1 \leq \sqrt{2m - \lambda_1^2}$ if λ_1 is positive and $\sqrt{2m-\lambda_1^2} \leq \lambda_1$ if λ_1 is negative.

Since λ_1 is always positive, we have $-\lambda_1 \leq \sqrt{2m - \lambda_1^2}$. Under this there are two cases:

$$\begin{aligned} \lambda_1^2 \leq (2m - \lambda_1^2) \quad &\text{if} \quad \lambda_1 \leq \sqrt{2m-\lambda_1^2}, \\ \lambda_1^2 \geq (2m - \lambda_1^2) \quad &\text{if} \quad \lambda_1 \geq \sqrt{2m-\lambda_1^2}. \end{aligned}$$

Thus,

$$\begin{aligned} \lambda_1 \leq \sqrt{m} \quad &\text{if} \quad \lambda_1 \leq \sqrt{2m-\lambda_1^2}, \\ \lambda_1 \geq \sqrt{m} \quad &\text{if} \quad \lambda_1 \geq \sqrt{2m-\lambda_1^2}. \end{aligned}$$

□

Note:1. It follows from the above lemma that

$$0 \leq \lambda_1 \leq \sqrt{m} \quad \text{if} \quad \lambda_1 \leq \sqrt{2m - \lambda_1^2},$$

$$\sqrt{m} \leq \lambda_1 \leq \sqrt{2m} \quad \text{if} \quad \lambda_1 \geq \sqrt{2m - \lambda_1^2}.$$

Lemma 2.2. *If G is a graph with n vertices and m edges then the largest eigenvalue, λ_1 of G satisfies*

$$|\lambda_1| \geq \frac{(n-1)|det(A)|^{\frac{2}{n(n-1)}}}{\sqrt{2m}}.$$

Proof. Obtain arithmetic and geometric mean for numbers $|\lambda_i||\lambda_j|$ for all $i \neq j$ $(i, j = 1, 2..., n)$. Since arithmetic mean is greater than are equal to geometric mean it follows that

$$\frac{\sum_{i\neq j} |\lambda_i||\lambda_j|}{n(n-1)} \geq \prod_{i\neq j} |\lambda_i||\lambda_j|^{\frac{1}{n(n-1)}}$$

$$\sum_{i\neq j} |\lambda_i||\lambda_j| \geq n(n-1) \prod |\lambda_i|^{\frac{2}{n(n-1)}}$$

$$\geq n(n-1)|det(A)|^{\frac{2}{n(n-1)}}$$

Thus

$$\begin{aligned} n(n-1)|det(A)|^{\frac{2}{n(n-1)}} &\leq \sum_{i\neq j} |\lambda_i||\lambda_j| \\ &\leq \sum_{j=1}^{n} \sqrt{2m}|\lambda_j| \\ &\leq \sum_{j=1}^{n} \sqrt{2m}|\lambda_1| \\ &\leq \sqrt{2m}n|\lambda_1| \end{aligned}$$

Hence, $|\lambda_1| \geq \frac{(n-1)|det(A)|^{\frac{2}{n(n-1)}}}{\sqrt{2m}}$. □

Corollary 2.1. *If G is a graph with n vertices and m edges then*

$$\mathcal{E}(G) \geq \frac{n(n-1)|det(A)|^{\frac{2}{n(n-1)}}}{\sqrt{2m}}.$$

Proof. Proof of this follows from $n(n-1)|det(A)|^{\frac{2}{n(n-1)}} \leq \sqrt{2m}\sum_{j=1}^{n}|\lambda_j|$ of previous lemma. □

Lemma 2.3. *Let G be a graph with n vertices and m edges. The smallest absolute eigenvalue satisfies*

$$|\lambda_n| \leq (2m)^{\frac{1}{4}}|det(A)|^{\frac{1}{2n}}.$$

Proof. We begin with $|det(A)| = |\lambda_1\lambda_2\cdots\lambda_n|$. Consider

$$\begin{aligned}(\sqrt{2m})^n|\lambda_1\lambda_2\cdots\lambda_n| &= \underbrace{\sqrt{2m}\sqrt{2m}\cdots\sqrt{2m}}_{(ntimes)}|\lambda_1||\lambda_2|\cdots|\lambda_n| \\ &\geq |\lambda_1|^2|\lambda_2|^2\cdots|\lambda_n|^2 \\ &\geq |\lambda_n|^2|\lambda_n|^2\cdots|\lambda_n|^2 \\ &= |\lambda_n|^{2n}.\end{aligned}$$

Thus $|\lambda_n| \leq (\sqrt{2m})^{\frac{1}{2}}|det(A)|^{\frac{1}{2n}}$. □

Remark 2.1. *Since $|det(A)| \leq (2m)^{\frac{n}{2}}$ so $|\lambda_n| \leq (\sqrt{2m})^{\frac{1}{2}}|det(A)|^{\frac{1}{2n}}$ implies $|\lambda_n| \leq (2m)^{\frac{3}{4}}$.*

3. Lower and upper bound for energy of graph

Theorem 3.1. *Let G be a graph with n vertices, m edges then $\mathcal{E}(G) \geq \sqrt{2m}$.*

Proof. The proof is simple and is follows from $\sum_{i=1}^{n}|\lambda_i|^2 \leq \sqrt{2m}\sum_{i=1}^{n}|\lambda_i|$. □

Theorem 3.2. *Let G be a graph with n vertices, m edges then $\mathcal{E}(G) \geq 2\sqrt{m}$.*

Proof. For $(n-1)$ absolute eigenvalues $|\lambda_2|, |\lambda_3|, \cdots, |\lambda_n|$ we know that

$$\sqrt{|\lambda_2|^2 + |\lambda_3|^2 + \cdots + |\lambda_n|^2} \leq |\lambda_2| + |\lambda_3| + \cdots + |\lambda_n|,$$

$$\sqrt{2m - |\lambda_1|^2} \leq \mathcal{E}(G) - |\lambda_1|.$$

Thus $\mathcal{E}(G) \geq |\lambda_1| + \sqrt{2m - |\lambda_1|^2}$.

Let $|\lambda_1| = x$ and $f(x) = x + \sqrt{2m - x^2}$. At maxima or minima when $f'(x) = 0$ which gives $1 - \frac{x}{\sqrt{2m-x^2}} = 0$. Hence the function attains maximum or minimum value at $x = \sqrt{m}$. At this point $f''(x) = -\frac{2m}{(2m-x^2)^{\frac{3}{2}}} = -\frac{2}{\sqrt{m}} < 0$, hence the function attains maximum value at this point. The maximum value $f(\sqrt{m}) = \sqrt{m} + \sqrt{2m - m}$ and $\mathcal{E}(G) \geq 2\sqrt{m}$. □

Theorem 3.3. *Let G be a graph with $n \geq 2$ vertices, m edges then*

$$\mathcal{E}(G) \geq \frac{5}{2\sqrt{2}}\sqrt{m}.$$

Proof. Consider

$$|\lambda_2|^2 + |\lambda_3|^2 + \cdots + |\lambda_n|^2 \leq \sqrt{2m}|\lambda_2| + \sqrt{2m}|\lambda_3| + \cdots + \sqrt{2m}|\lambda_n|$$
$$2m - |\lambda_1|^2 \leq \sqrt{2m}(\mathcal{E}(G) - |\lambda_1|)$$

So, $\mathcal{E}(G) \geq |\lambda_1| + \frac{2m-|\lambda_1|^2}{\sqrt{2m}} = |\lambda_1| + \sqrt{2m} - \frac{|\lambda_1|^2}{\sqrt{2m}}$.

Let $g(x) = x + \sqrt{2m} - \frac{x^2}{\sqrt{2m}}$ where $x = |\lambda_1|$. Then $g'(x) = 1 - \frac{2x}{\sqrt{2m}}$ and $g''(x) = -\frac{2}{\sqrt{2m}} < 0$. At maximum or minimum $g'(x) = 0$, which gives $1 - \frac{2x}{\sqrt{2m}} = 0$. Thus $g(x)$ attains maximum value at $x = \sqrt{\frac{m}{2}}$. Maximum value $g\left(\sqrt{\frac{m}{2}}\right) = \sqrt{\frac{m}{2}} + \sqrt{2m} - \frac{\frac{m}{2}}{\sqrt{2m}}$.

$$\therefore \mathcal{E}(G) \geq \frac{5}{2\sqrt{2}}\sqrt{m}.$$

□

Theorem 3.4. *Let G be a graph with $n \geq 2$ vertices, m edges and $|\lambda_1|^2 + |\lambda_n|^2 \neq 2m$ then*

$$\mathcal{E}(G) \geq 2.386\sqrt{m} \quad \textit{if} \quad \lambda_1 \leq \sqrt{2m - \lambda_1^2},$$
$$\mathcal{E}(G) \geq 2\sqrt{m} \quad \textit{if} \quad \lambda_1 \geq \sqrt{2m - \lambda_1^2}.$$

Proof. For $(n-2)$ absolute eigenvalues $|\lambda_2|, |\lambda_3|, \cdots, |\lambda_{n-1}|$ we know that

$$\sqrt{|\lambda_2|^2 + |\lambda_3|^2 + \cdots + |\lambda_{n-1}|^2} \leq |\lambda_2| + |\lambda_3| + \cdots + |\lambda_{n-1}|$$

and

$$\sqrt{2m - |\lambda_1|^2 - |\lambda_n|^2} \leq \mathcal{E}(G) - |\lambda_1| - |\lambda_n|.$$

Thus $\mathcal{E}(G) \geq |\lambda_1| + |\lambda_n| + \sqrt{2m - |\lambda_1|^2 - |\lambda_n|^2}$. Equality holds if if G is $K_{m,n}$.

Let $|\lambda_1| = x$, $|\lambda_n| = y$ and $\phi(x,y) = x + y + \sqrt{2m - x^2 - y^2}$. Using partial differentiation we maximize the function by finding $\phi_x(x,y)$, $\phi_y(x,y)$, $\phi_{xx}(x,y)$, $\phi_{yy}(x,y)$, $\phi_{xy}(x,y)$ and $\Delta = \phi_{xx}\phi_{yy} - \phi_{xy}^2$. Also,

$$\phi_x = 1 - \frac{x}{\sqrt{2m-x^2-y^2}},\ \phi_y = 1 - \frac{y}{\sqrt{2m-x^2-y^2}},\ \phi_{xx} = -\frac{(2m-x^2)}{(2m-x^2-y^2)^{\frac{3}{2}}} \leq 0,$$
$$\phi_{yy} = -\frac{(2m-y^2)}{(2m-x^2-y^2)^{\frac{3}{2}}},\ \phi_{xy} = \frac{xy}{(2m-x^2-y^2)^{\frac{3}{2}}},\ \Delta = \frac{2m}{(2m-x^2-y^2)^2}.$$

At maxima or minimum $\phi_x(x) = 0$ and $\phi_y(y) = 0$ which gives $\sqrt{2m - x^2 - y^2} - x = 0$ and $\sqrt{2m - x^2 - y^2} - y = 0$. Solving these equations gives $x = y = \sqrt{\frac{2m}{3}}$. Since $|\lambda_1|^2 + |\lambda_n|^2 \neq 2m$, at these points $\Delta = \frac{9}{2m} > 0$.

Thus we can conclude that $\phi(x, y)$ takes maximum value at $x = y = \frac{\sqrt{2m}}{\sqrt{3}}$. Maximum value $\phi\Big(\frac{\sqrt{2m}}{\sqrt{3}}, \frac{\sqrt{2m}}{\sqrt{3}}\Big) = \frac{\sqrt{2m}}{\sqrt{3}} + \frac{\sqrt{2m}}{\sqrt{3}} + \frac{\sqrt{2m}}{\sqrt{3}} = \sqrt{6m}$. But $\phi(x, y)$ decreases in the interval $\sqrt{\frac{2}{3}m} \leq x \leq \sqrt{m}$ and $\sqrt{\frac{2}{3}m} \leq y \leq \sqrt{m}$. The above condition is true if $x = \lambda_1$ satisfies $\lambda_1 \leq \sqrt{2m - \lambda_1^2}$. If $\lambda_1 \geq \sqrt{2m - \lambda_1^2}$ then we have $\sqrt{\frac{2}{3}m} \leq \sqrt{m} \leq x$ and $\sqrt{\frac{2}{3}m} \leq y \leq \sqrt{m}$. Hence if $\lambda_1 \leq \sqrt{2m - \lambda_1^2}$ then at $x = \sqrt{m}$, $\phi(x, y) \geq \phi(\sqrt{m}, \sqrt{\frac{2}{3}m})$ which implies $\mathcal{E}(G) \geq \sqrt{m}\Big(1 + \sqrt{\frac{2}{3}} + \sqrt{\frac{1}{3}}\Big) = 2.386\sqrt{m}$. If $\lambda_1 \geq \sqrt{2m - \lambda_1^2}$ then at $x = \sqrt{m}$, $\phi(x, y) \geq \phi(\sqrt{m}, \sqrt{m})$ which implies $\mathcal{E}(G) \geq 2\sqrt{m}$. In conclusion,

$$\mathcal{E}(G) \geq 2.386\sqrt{m} \quad if \quad \lambda_1 \leq \sqrt{2m - \lambda_1^2}.$$
$$\mathcal{E}(G) \geq 2\sqrt{m} \quad if \quad \lambda_1 \geq \sqrt{2m - \lambda_1^2}.$$

□

Remark 3.1. *From the above theorems we have,*

1. $\frac{5}{2\sqrt{2}}\sqrt{m} \leq \sqrt{2m} \leq 2.386\sqrt{m} \leq \mathcal{E}(G)$ *if* $\lambda_1 \leq \sqrt{2m - \lambda_1^2}$*; and*
2. $\frac{5}{2\sqrt{2}}\sqrt{m} \leq \sqrt{2m} \leq 2\sqrt{m} \leq \mathcal{E}(G)$ *if* $\lambda_1 \geq \sqrt{2m - \lambda_1^2}$. .

The following theorem gives an upper bound for energy of graph when $\lambda_1 \leq \sqrt{2m - \lambda_1^2}$.

Theorem 3.5. *Let G be a graph with $n \geq 2$ vertices, m edges. If λ_1 satisfies $\lambda_1 \leq \sqrt{2m - \lambda_1^2}$, then*

$$\mathcal{E}(G) \leq \sqrt{m(n^2 - n + 2)}.$$

Proof. Consider $\Big(\mathcal{E}(G)\Big)^2 = \Big(\sum_{i=1}^{n} |\lambda_i|\Big)^2 = \sum_{i=1}^{n} |\lambda_i|^2 + \underbrace{\sum_{i\neq j} |\lambda_i||\lambda_j|}_{n(n-1)\ terms}$. But

$$\sum_{i\neq j} |\lambda_i||\lambda_j| \leq \sum |\lambda_1||\lambda_1| = n(n-1)|\lambda_1|^2$$
$$\therefore \Big(\mathcal{E}(G)\Big)^2 \leq 2m + n(n-1)|\lambda_1|^2.$$

Since $\lambda_1 \leq \sqrt{2m - \lambda_1^2}$ so $|\lambda_1| \leq \sqrt{m}$ and hence we have $\mathcal{E}(G) \leq \sqrt{m(n^2 - n + 2)}$.

□

4. Bounds for energy of graph

Theorem 4.1. *Let G be a graph with n vertices and m edges then*

$$\frac{\sqrt{2m}(n-1-\sqrt{(n-1)^2+4})}{2} \leq \mathcal{E}(G) \leq \frac{\sqrt{2m}(n-1+\sqrt{(n-1)^2+4})}{2}.$$

Proof. Consider

$$\begin{aligned}\Big(\mathcal{E}(G)\Big)^2 &= \Big(\sum_{i=1}^{n}|\lambda_i|\Big)^2 \\ &= \sum_{i=1}^{n}|\lambda_i|^2 + \underbrace{\sum_{i\neq j}|\lambda_i||\lambda_j|}_{n(n-1)\ terms} \\ &\leq 2m + \sqrt{2m}\Big(\sum_{i=1}^{n}|\lambda_i|\Big)(n-1) \\ \Big(\mathcal{E}(G)\Big)^2 &\leq 2m + \sqrt{2m}\Big(\mathcal{E}(G)\Big)(n-1) \\ \Big(\mathcal{E}(G)\Big)^2 &- \sqrt{2m}\Big(\mathcal{E}(G)\Big)(n-1) - 2m \leq 0.\end{aligned}$$

The roots of the equation $x^2 - \sqrt{2m}(n-1)x - 2m = 0$ are

$$x = m_1 = \frac{\sqrt{2m}(n-1-\sqrt{(n-1)^2+4})}{2}$$

and

$$x = m_2 = \frac{\sqrt{2m}(n-1+\sqrt{(n-1)^2+4})}{2}.$$

Hence, the equation implies $(x-m_1)(x-m_2) \leq 0$, which is true for $x \leq m_1$ and $x \geq m_2$ or $x \geq m_1$ and $x \leq m_2$. The only inequality which satisfy is $m_1 \leq \mathcal{E}(G) \leq m_2$. So,

$$\Rightarrow \frac{\sqrt{2m}(n-1-\sqrt{(n-1)^2+4})}{2} \leq \mathcal{E}(G) \leq \frac{\sqrt{2m}(n-1+\sqrt{(n-1)^2+4})}{2}.$$

□

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