# The Spectral Moments and Energy of Graphs 

Rao Li<br>Dept. of Mathematical Sciences<br>University of South Carolina Aiken<br>Aiken, SC 29801, USA<br>raol@usca.edu


#### Abstract

The energy of a graph is defined as the sum of the absolute values of its eigenvalues. In this paper, we obtain an upper bound for the energy of a graph that involves its moments.


Mathematics Subject Classification: 05C50
Keywords: Eigenvalues, Energy and moments of a graph

## 1. Introduction

We consider only finite undirected graphs without loops or multiple edges. Notation and terminology not defined here follow that in [1]. Throught this paper, $G$ will be always a graph of order $n$ and size $m$. We use $V(G):=$ $\left\{v_{1}, v_{2}, \ldots v_{n}\right\}$ to denote the vertex set of $G$ and $d\left(v_{i}\right)$ or $d_{i}$, where $1 \leq i \leq n$, to denote the degree of vertex $v_{i}$. For each $1 \leq i \leq n$, the 2 - degree of $v_{i}$, denoted $t\left(v_{i}\right)$ or $t_{i}$, is defined as the sum of degrees of the vertices adjacent to $v_{i}$, the average degree of $v_{i}$ is defined as $t_{i} / d_{i}$, and $\sigma\left(v_{i}\right)$ or $\sigma_{i}$ is defined as the sum of the 2 - degrees of vertices adjacent to $v_{i}$. We define $\Sigma_{k}(G)$ as $\sum_{i=1}^{n} d_{i}^{k}$. A bipartite graph $G=(X, Y ; E)$ is $(a, b)$ - semiregular if there exist two constants $a$ and $b$ such that each vertex in $X$ has degree $a$ and each vertex in $Y$ has degree $b$. A bipartite graph $G=(X, Y ; E)$ is $\left(p_{x}, p_{y}\right)$ - pseudo semiregular if there exist two constants $p_{x}$ and $p_{y}$ such that each vertex in $X$ has average degree $p_{x}$ and each vertex in $Y$ has average degree $p_{y}$. The eigenvalues $\mu_{1}(G) \geq \mu_{2}(G) \geq \ldots \geq \mu_{n}(G)$ of the adjacency matrix $A(G)$ of $G$ are called the eigenvalues of the graph $G$. The $k$ th - spectral moments, denoted $M_{k}(G)$ or $M_{k}$, of $G$ is defined as $\sum_{i=1}^{n} \mu_{i}^{k}$ (see [6]). The energy of a graph $G$, denoted $E(G)$, is defined as $E(G)=\sum_{i=1}^{n}\left|\mu_{i}\right|$. This concept was introduced by Gutman in [4] and more information and background on the energy of graphs can be found in [5]. In 1971, McClelland [11] proved that $E(G) \leq \sqrt{2 m n}$, the first upper bound for $E(G)$. Since then, more upper bounds for $E(G)$ have
been found and some of them can be found in the following theorems.
Theorem 1 [8]. Let $G$ be a graph on $n$ vertices and $m$ edges. If $2 m \geq n$, then the inequality

$$
\begin{equation*}
E(G) \leq \frac{2 m}{n}+\sqrt{(n-1)\left[2 m-\left(\frac{2 m}{n}\right)^{2}\right]} \tag{1}
\end{equation*}
$$

holds. Moreover, equality holds if and only if $G$ is either $\frac{n}{2} K_{2}, K_{n}$, or a noncomplete connected strongly regular graph with two non-trivial eigenvalues with absolute value $\sqrt{\left(2 m-\left(\frac{2 m}{n}\right)^{2}\right) /(n-1)}$. If $2 m \leq n$, then the inequality $E(G) \leq 2 m$ holds. Moreover, equality holds if and only if $G$ is disjoint union of edges and isolated vertices.

Theorem 2 [9]. If $2 m \geq n$ and $G$ is a bipartite graph with $n>2$ vertices and $m$ edges, then the inequality

$$
\begin{equation*}
E(G) \leq 2\left(\frac{2 m}{n}\right)+\sqrt{(n-2)\left[2 m-2\left(\frac{2 m}{n}\right)^{2}\right]} \tag{2}
\end{equation*}
$$

holds. Moreover, equality holds if and only if at least one of the following statements holds:
(1) $n=2 m$ and $G=m K_{2}$.
(2) $n=2 t, m=t^{2}$, and $G=K_{t, t}$.
(3) $n=2 \nu, 2 \sqrt{m}<n<2 m$, and $G$ is the incidence graph of a symmetric $2-(\nu, k, \lambda)-$ design with $k=\frac{2 m}{n}$ and $\lambda=\frac{k(k-1)}{\nu-1}$.

Theorem 1 and Theorem 2 were generalized by several authors (see [13] [12]) and the latest ones are the following Theorem 3 and Theorem 4 proved by Liu, Lu, and Tian.

Theorem 3 [10]. Let $G$ be a non-empty graph on $n$ vertices, $m$ edges. Then the inequality

$$
\begin{equation*}
E(G) \leq \sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}+\sqrt{(n-1)\left(2 m-\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}\right)} \tag{3}
\end{equation*}
$$

holds. Moreover, equality in (3) holds if and only if $G$ is either $\frac{n}{2} K_{2}, K_{n}$, or a non-bipartite connected graph satifying $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ and has three distinct eigenvalues $\left(p, \sqrt{\frac{2 m-p^{2}}{n-1}},-\sqrt{\frac{2 m-p^{2}}{n-1}}\right)$, where $p=\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}>$ $\sqrt{\frac{2 m}{n}}$.

Theorem 4 [10]. Let $G=(X, Y)$ be a non-empty bipartite graph with $n>2$ vertices and $m$ edges. Then the inequality

$$
\begin{equation*}
E(G) \leq 2 \sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}+\sqrt{(n-2)\left(2 m-2 \frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}\right)} \tag{4}
\end{equation*}
$$

holds. Moreover, equality in (4) holds if and only if $G$ is either $\frac{n}{2} K_{2}, K_{r_{1}, r_{2}} \cup$ $\left(n-r_{1}-r_{2}\right) K_{1}$, where $r_{1} r_{2}=m$, or a connected bipartite graph with $V=$ $\left\{v_{1}, v_{2}, \ldots, v_{s}\right\} \cup\left\{v_{s+1}, v_{s+2}, \ldots, v_{n}\right\}$ such that $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}$ and $\frac{\sigma_{s+1}}{t_{s+1}}=$ $\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$, and has four distinct eigenvalues $\left(\sqrt{p_{x} p_{y}}, \sqrt{\frac{2 m-2 p_{x} p_{y}}{n-2}},-\sqrt{\frac{2 m-2 p_{x} p_{y}}{n-2}},-\sqrt{p_{x} p_{y}}\right)$, where $p_{x}=\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}, p_{y}=\frac{\sigma_{s+1}}{t_{s+1}}=\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ and $\sqrt{p_{x} p_{y}}>\sqrt{\frac{2 m}{n}}$.

Motivated by Theorem 3 and Theorem 4 above, we in this paper prove the following theorems.

Theorem 5. Let $G$ be a non-empty graph on $n$ vertices. If $\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}} \geq$ $\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$, where $k$ is a positive integer, then the inequality

$$
\begin{equation*}
E(G) \leq \sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}+(n-1)^{\frac{2 k-1}{2 k}}\left(M_{2 k}-\left(\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}\right)^{k}\right)^{\frac{1}{2 k}} \tag{5}
\end{equation*}
$$

holds. Moreover, equality in (5) holds if and only if $G$ is either $\frac{n}{2} K_{2}, K_{n}$, or a non-bipartite connected graph satifying $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ and has three distinct eigenvalues $\left(p,\left(\frac{M_{2 k}-p^{2 k}}{n-1}\right)^{\frac{1}{2 k}},-\left(\frac{M_{2 k}-p^{2 k}}{n-1}\right)^{\frac{1}{2 k}}\right)$, where $p=\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=$ $\frac{\sigma_{n}}{t_{n}}>\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$.

Theorem 6. Let $G=(X, Y)$ be a non-empty bipartite graph with $n>2$ vertices amd $m$ edges. If $\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}} \geq\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$, where $k$ is a positive integer, then the inequality

$$
\begin{equation*}
E(G) \leq 2 \sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}+(n-2)^{\frac{2 k-1}{2 k}}\left(M_{2 k}-2\left(\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}\right)^{k}\right)^{\frac{1}{2 k}} \tag{6}
\end{equation*}
$$

holds. Moreover, equality in (6) holds if and only if $G$ is either $\frac{n}{2} K_{2}, K_{r_{1}, r_{2}} \cup$ $\left(n-r_{1}-r_{2}\right) K_{1}$, where $r_{1} r_{2}=m$, or a connected bipartite graph with $V=$ $\left\{v_{1}, v_{2}, \ldots, v_{s}\right\} \cup\left\{v_{s+1}, v_{s+2}, \ldots, v_{n}\right\}$ such that $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}$ and $\frac{\sigma_{s+1}}{t_{s+1}}=$ $\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$, and has four distinct eigenvalues $\left(\sqrt{p_{x} p_{y}},\left(\frac{M_{2 k}-2\left(p_{x} p_{y}\right)^{k}}{n-2}\right)^{\frac{1}{2 k}}\right.$, $\left.-\left(\frac{M_{2 k}-2\left(p_{x} p_{y}\right)^{k}}{n-2}\right)^{\frac{1}{2 k}},-\sqrt{p_{x} p_{y}}\right)$, where $p_{x}=\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}, p_{y}=\frac{\sigma_{s+1}}{t_{s+1}}=$
$\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ and $\sqrt{p_{x} p_{y}}>\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$.
Notice that $\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}} \geq\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$ is always true when $k=1$ (see [10]) and $M_{2}=2 m$. Thus if we let $k=1$ in Theorem 5 and Theorem 6 , then they become Theorem 3 and Theorem 4 respectively.

Let $q$ be the number of quadrangles in a graph $G$. Then $M_{4}(G)=2 \sum_{i=1}^{n} d_{i}^{2}-$ $2 m+8 q$ (see [6]). Thus if we let $k=2$ and replace $M_{4}$ by $2 \sum_{i=1}^{n} d_{i}^{2}-2 m+8 q$ in Theorem 5 and Theorem 6 then we can obtain upper bounds for general graphs and bipartite graphs which satisfy respectively the conditions in Theorem 5 and Theorem 6.

## 2. Lemmas

In order to prove Theorem 5 and Theorem 6, we need the following results as our lemmas. The first one is a theorem proved by Hong and Zhang in [7].

Lemma $1[7]$. Let $G$ be a simple connected graph of order $n$. Then

$$
\mu_{1} \geq \sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}
$$

with equality if and only if $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ or $G$ is a bipartite graph with $V=\left\{v_{1}, v_{2}, \ldots, v_{s}\right\} \cup\left\{v_{s+1}, v_{s+2}, \ldots, v_{n}\right\}$ such that $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}$ and $\frac{\sigma_{s+1}}{t_{s+1}}=\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$.

In fact, the above Hong and Zhang's theorem can be slightly strengthened to the following Lemma $1^{\prime}$. Notice that Lemma $1^{\prime}$ has been used by Liu, Lu, and Tian in [10] to obtain their results.

Lemma 1'. Let $G$ be a non-empty simple graph of order $n$. Then

$$
\mu_{1} \geq \sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}
$$

with equality if and only if $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ with $\mu_{1}=\frac{\sigma_{1}}{t_{1}}$ or $G$ is a bipartite graph with $V=\left\{v_{1}, v_{2}, \ldots, v_{s}\right\} \cup\left\{v_{s+1}, v_{s+2}, \ldots, v_{n}\right\}$ such that $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=$ $\frac{\sigma_{s}}{t_{s}}$ and $\frac{\sigma_{s+1}}{t_{s+1}}=\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ with $\mu_{1}=\sqrt{p_{x} p_{y}}$, where $p_{x}=\frac{\sigma_{1}}{t_{1}}$ and $p_{y}=\frac{\sigma_{n}}{t_{n}}$.

The following Lemma 2 and Lemma 3 can be found in [3] and [2] respectively.

Lemma 2 [3]. A graph $G$ has only one distinct eigenvalue if and only if $G$ is an empty graph. A graph $G$ has two distinct eigenvalues $\mu_{1}>\mu_{2}$ with multiplicities $s_{1}$ and $s_{2}$ if and only if $G$ is the direct sum of $s_{1}$ complete graphs of order $\mu_{1}+1$. In this case, $\mu_{2}=-1$ and $s_{2}=s_{1} \mu_{1}$.

Lemma 3 [2]. Let $G$ be a graph with $m$ edges. Then $E(G) \geq 2 \sqrt{m}$ with equality if and only if $G$ is a complete bipartite graph plus arbitrarily many isolated vertices.

## 3. Proofs

Proof of Theorem 5. Let $G$ be a graph satisfying the conditions in Theorem 9. Set $\alpha:=\frac{1}{2 k}$ and $\beta:=1-\alpha$. By the Hölder inequality, we have that

$$
\sum_{i=2}^{n}\left|\mu_{i}\right| \leq\left(\sum_{i=2}^{n} 1^{\frac{1}{\beta}}\right)^{\beta}\left(\sum_{i=2}^{n}\left|\mu_{i}\right|^{\frac{1}{\alpha}}\right)^{\alpha} .
$$

Therefore

$$
E(G)=\sum_{i=1}^{n}\left|\mu_{i}\right| \leq \mu_{1}+(n-1)^{\beta}\left(M_{2 k}-\mu_{1}^{2 k}\right)^{\frac{1}{2 k}}
$$

Consider the function $f(x)=x+(n-1)^{\beta}\left(M_{2 k}-x^{2 k}\right)^{\frac{1}{2 k}}$. It can be verified that $f(x)$ is decreasing when $\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}} \leq x \leq M_{2 k}^{\frac{1}{2 k}}$.

From Lemma $1^{\prime}$ and the assumption that

$$
\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}} \geq\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}
$$

we have that

$$
E(G) \leq f\left(\mu_{1}\right) \leq f\left(\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}\right)
$$

Therefore Inequality (5) is proved.
If $G$ is $\frac{n}{2} K_{2}$, then $\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}=1=\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$ and both sides of Inequality (5) are equal to $n$.

If $G$ is $K_{n}$, then $\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}=n-1$. From $(n-1) \geq\left(\frac{(n-1)^{2 k}+(n-1)}{n}\right)^{\frac{1}{2 k}}$, we have $\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}=(n-1) \geq\left(\frac{(n-1)^{2 k}+(n-1)}{n}\right)^{\frac{1}{2 k}}=\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$ and both sides of Inequality (5) are equal to $2(n-1)$.

If $G$ is a non-bipartite connected graph satisfying $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ and has three distinct eigenvalues $\left(p,\left(\frac{M_{2 k}-p^{2 k}}{n-1}\right)^{\frac{1}{2 k}},-\left(\frac{M_{2 k}-p^{2 k}}{n-1}\right)^{\frac{1}{2 k}}\right)$, where $p=$ $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}>\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$, then both sides of Inequality (5) are equal to $p+(n-1)\left(\frac{M_{2 k}-p^{2 k}}{n-1}\right)^{\frac{1}{2 k}}$.

Now suppose that Inequality (5) becomes an equality. Then we have that $\left|\mu_{2}\right|=\left|\mu_{3}\right|=\cdots=\left|\mu_{n}\right|=\left(\frac{M_{2 k}-\mu_{1}^{2 k}}{n-1}\right)^{\frac{1}{2 k}}$ and $\mu_{1}=\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}$. By Lemma $1^{\prime}$, we have that $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ or $G$ is a bipartite graph with $V=$ $\left\{v_{1}, v_{2}, \ldots, v_{s}\right\} \cup\left\{v_{s+1}, v_{s+2}, \ldots, v_{n}\right\}$ such that $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}$ and $\frac{\sigma_{s+1}}{t_{s+1}}=$ $\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$. Since $G$ is a non-empty graph, Lemma 2 implies that $G$ has at least two distinct eigenvalues. Hence we just have the following possible cases.

Case 1. $G$ has two distinct eigenvalues
If the two distinct eigenvalues of $G$ have the same absolute values, then Lemma 2 implies that $\mu_{1}=\left|\mu_{2}\right|=\cdots=\left|\mu_{n}\right|=1$. Since $\sum_{i=1}^{n} \mu_{i}=0$, the multiplicity $s_{1}$ of $\mu_{1}=1$ must be equal to $\frac{n}{2}$. Hence $G$ is the direct sum of $s_{1}=\frac{n}{2}$ complete graphs of order $\mu_{1}+1=2$. Namely, $G$ is $\frac{n}{2} K_{2}$.

If the two distinct eigenvalues of $G$ have different absolute values, then Lemma 2 implies that $\mu_{2}=\cdots=\mu_{n}=-1$. Since $\sum_{i=1}^{n} \mu_{i}=0, \mu_{1}=n-1$ and the multiplicity $s_{1}$ of $\mu_{1}$ is 1 . Hence $G$ is the direct sum of $s_{1}=1$ complete graph of order $\mu_{1}+1=n$. Namely, $G$ is $K_{n}$.

Case 2. $G$ has three distinct eigenvalues
Since $G$ has three distinct eigenvalues, there exists an integer $r$ such that $\mu_{1}>\mu_{2}=\cdots=\mu_{r}>0>\mu_{r+1}=\cdots=\mu_{n}$ and $\mu_{2}=-\mu_{n}$. Hence $\mu_{1} \neq-\mu_{n}$ and $G$ cannot be a bipartite graph. From $\mu_{1}=\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}$ and $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=$ $\frac{\sigma_{n}}{t_{n}}$, we have that $\mu_{1}=\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$. Since $\mu_{1}>\mu_{i}$, for each $i$ with $2 \leq i \leq n, G$ must be connected. Set $p:=\mu_{1}$. Then $G$ has three distinct eigenvalues $\left(p,\left(\frac{M_{2 k}-p^{2 k}}{n-1}\right)^{\frac{1}{2 k}},-\left(\frac{M_{2 k}-p^{2 k}}{n-1}\right)^{\frac{1}{2 k}}\right)$, where $p=\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}>$ $\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$.

Proof of Theorem 6. Let $G$ be a graph satisfying the conditions in Theorem 10. Then $\mu_{1}=-\mu_{n}$. Set $\alpha:=\frac{1}{2 k}$ and $\beta:=1-\alpha$. By the Hölder inequality, we have that

$$
\sum_{i=2}^{n-1}\left|\mu_{i}\right| \leq\left(\sum_{i=2}^{n-1} 1^{\frac{1}{\beta}}\right)^{\beta}\left(\sum_{i=2}^{n-1}\left|\mu_{i}\right|^{\frac{1}{\alpha}}\right)^{\alpha}
$$

Therefore

$$
E(G)=\sum_{i=1}^{n}\left|\mu_{i}\right| \leq 2 \mu_{1}+(n-2)^{\beta}\left(M_{2 k}-2 \mu_{1}^{2 k}\right)^{\frac{1}{2 k}} .
$$

Consider the function $f(x)=2 x+(n-2)^{\beta}\left(M_{2 k}-2 x^{2 k}\right)^{\frac{1}{2 k}}$. It can be verified that $f(x)$ is decreasing when $\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}} \leq x \leq M_{2 k}^{\frac{1}{2 k}}$.

From Lemma $1^{\prime}$ and the assumption that

$$
\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}} \geq\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}},
$$

we have that

$$
E(G) \leq f\left(\mu_{1}\right) \leq f\left(\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}\right)
$$

Therefore Inequality (6) is proved.
If $G$ is $\frac{n}{2} K_{2}$, then $\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}=1=\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$ and both sides of Inequality (6) are equal to $n$.

If $G$ is $K_{r_{1}, r_{2}} \cup\left(n-r_{1}-r_{2}\right) K_{1}$, where $r_{1} r_{2}=m$, then $\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}=\sqrt{r_{1} r_{2}} \geq$ $\left.\left(\frac{2\left(r_{1} r_{2}\right)^{k}}{n}\right)^{\frac{1}{2 k}}\right)=\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$ and both sides of Inequality (6) are equal to $2 \sqrt{r_{1} r_{2}}$.

If $G$ is a connected bipartite graph with $V=\left\{v_{1}, v_{2}, \ldots, v_{s}\right\} \cup\left\{v_{s+1}\right.$, $\left.v_{s+2}, \ldots, v_{n}\right\}$ such that $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}$ and $\frac{\sigma_{s+1}}{t_{s+1}}=\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$, and has four distinct eigenvalues $\left(\sqrt{p_{x} p_{y}},\left(\frac{M_{2 k}-2\left(p_{x} p_{y}\right)^{k}}{n-2}\right)^{\frac{1}{2 k}},-\left(\frac{M_{2 k}-2\left(p_{x} p_{y}\right)^{k}}{n-2}\right)^{\frac{1}{2 k}},-\sqrt{p_{x} p_{y}}\right)$, where $p_{x}=\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}, p_{y}=\frac{\sigma_{s+1}}{t_{s+1}}=\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ and $\sqrt{p_{x} p_{y}}>$ $\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$, then both sides of Inequality (6) are equal to $2 p+(n-2)\left(\frac{M_{2 k}-2 p^{2 k}}{n-2}\right)^{\frac{1}{2 k}}$, where $p=\sqrt{p_{x} p_{y}}$.

Now suppose that Inequality (6) becomes an equality. Then we have that $\left|\mu_{2}\right|=\left|\mu_{3}\right|=\cdots=\left|\mu_{n-1}\right|=\left(\frac{M_{2 k}-2 \mu_{1}^{2 k}}{n-2}\right)^{\frac{1}{2 k}}$ and $\mu_{1}=-\mu_{n}=\sqrt{\frac{\sum_{i=1}^{n} \sigma_{i}^{2}}{\sum_{i=1}^{n} t_{i}^{2}}}$. By Lemma $1^{\prime}$, we have that $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ or $G$ is a bipartite graph with $V=\left\{v_{1}, v_{2}, \ldots, v_{s}\right\} \cup\left\{v_{s+1}, v_{s+2}, \ldots, v_{n}\right\}$ such that $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}$ and $\frac{\sigma_{s+1}}{t_{s+1}}=\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ with $\mu_{1}=\sqrt{p_{x} p_{y}}$, where $p_{x}=\frac{\sigma_{1}}{t_{1}}$ and $p_{y}=\frac{\sigma_{n}}{t_{n}}$. Since $G$ is a non-empty graph, Lemma 2 implies that $G$ has at least two distinct eigenvalues. Hence we just have the following possible cases.

Case 1. $G$ has two distinct eigenvalues with the same absolute values

Then Lemma 2 implies that $\mu_{1}=-\mu_{n}=\left|\mu_{2}\right|=\cdots=\left|\mu_{n-1}\right|=1$. Since $\sum_{i=1}^{n} \mu_{i}=0$, the multiplicity $s_{1}$ of $\mu_{1}=1$ must be equal to $\frac{n}{2}$. Hence $G$ is the direct sum of $s_{1}=\frac{n}{2}$ complete graphs of order $\mu_{1}+1=2$. Namely, $G$ is $\frac{n}{2} K_{2}$.

Case 2. $G$ has three distinct eigenvalues
Since $G$ is a bipartite graph, we must have that $\mu_{1}=-\mu_{n} \neq 0$ and $\mu_{2}=$ $\cdots=\mu_{n-1}=0$. Thus $E(G)=2 \mu_{1}$. From Lemma 3, we have that $2 \mu_{1} \geq 2 \sqrt{m}$. Thus $2 \mu_{1}^{2} \geq 2 m$. Notice that $2 m=\sum_{i=1}^{n} \mu_{i}^{2}=2 \mu_{1}^{2}$. Therefore $\mu_{1}=\sqrt{m}$ and $E(G)=2 \sqrt{m}$. Hence by Lemma $3 G$ is a complete bipartite graph plus arbitrarily many isolated vertices. Namely, there exist integers $r_{1} \geq 1$ and $r_{2} \geq 1$ such that $G$ is $K_{r_{1}, r_{2}} \cup\left(n-r_{1}-r_{2}\right) K_{1}$, where $r_{1} r_{2}=m$.

Case 3. $G$ has four distinct eigenvalues
Since $\mu_{1}=-\mu_{n},\left|\mu_{2}\right|=\cdots=\left|\mu_{n-1}\right|$, and $G$ has four distinct eigenvalues, the multiplicity of $\mu_{1}$ must be one. Hence we have by Lemma $1^{\prime}$ that $G$ is a connected bipartite graph with $V=\left\{v_{1}, v_{2}, \ldots, v_{s}\right\} \cup\left\{v_{s+1}, v_{s+2}, \ldots, v_{n}\right\}$ such that $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}$ and $\frac{\sigma_{s+1}}{t_{s+1}}=\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$, and has four distinct eigenvalues $\left(\sqrt{p_{x} p_{y}},\left(\frac{M_{2 k}-2\left(p_{x} p_{y}\right)^{k}}{n-2}\right)^{\frac{1}{2 k}},-\left(\frac{M_{2 k}-2\left(p_{x} p_{y}\right)^{k}}{n-2}\right)^{\frac{1}{2 k}},-\sqrt{p_{x} p_{y}}\right)$, where $p_{x}=$ $\frac{\sigma_{1}}{t_{1}}=\frac{\sigma_{2}}{t_{2}}=\cdots=\frac{\sigma_{s}}{t_{s}}, p_{y}=\frac{\sigma_{s+1}}{t_{s+1}}=\frac{\sigma_{s+2}}{t_{s+2}}=\cdots=\frac{\sigma_{n}}{t_{n}}$ and $\sqrt{p_{x} p_{y}}>\left(\frac{M_{2 k}}{n}\right)^{\frac{1}{2 k}}$.

## References

[1] J. A. Bondy and U. S. R. Murty, Graph Theory with Applications, Macmillan, London and Elsevier, New York (1976).
[2] G. Caporossi, D. Cvetković, I. Gutman and P. Hansen, Variable beighbourhood search for extremal graphs, 2. Finding graphs with extremal energy, J. Chem. Info. Comput. Sci. 39 (1999) 984 - 996.
[3] D. Cvetković, M. Doob and H. Sachs, Spectra of Graphs - Theory and Applications, Academic Press, New York, 1980.
[4] I. Gutman, The energy of a graph, Berichte der Mathematisch - Statistischen Sektion im Forschungszentrum Graz 103 (1978) 1-12.
[5] I. Gutman, The energy of a graph, in: A. Betten, A. Kohnert, R. Laue, andA. Wassermann (Eds.), Algebraic Combinatorics and Applications, Springer - Verlag, Berlin, 2001, pp. 196 - 211.
[6] I. Gutman, On graphs whose energy exceeds the number of vertices, to appear in Linear Algebra Appl..
[7] Y. Hong and X. Zhang, Sharp upper and lower bounds for largest eigenvalue of the Laplacian matrices of trees, Discrete Math. 296 (2005) 187 197.
[8] J. H. Koolen and V. Moulton, Maximal energy graphs, Adv. Appl. Math. 26 (2001) $47-52$.
[9] J. H. Koolen and V. Moulton, Maximal energy bipartite graphs, Graphs Combin. 19 (2003) 131-135.
[10] H. Liu, M. Lu, and F. Tian, Some upper bounds for the energy of graphs, J. Mathematical Chem. 41 (2007) 45-57.
[11] B. J. McClelland, Properties of the latent roots of a matrix: The estimation of pi - electron energies, J. Chem. Phys. 54 (1971) $640-643$.
[12] A. Yu, M. Lu, and F. Tian, New upper bounds for the energy of graphs, MATCH Commun. Math. Comput. Chem. 53 (2005) 441 - 448.
[13] B. Zhou, Energy of graphs, MATCH Commun. Math. Comput. Chem. 51 (2004) 111 - 118.

Received: April, 2009

