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# On the spectral radius, $k$-degree and the upper bound of energy in a graph

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**Abstract:**

Let $G$ be a simple graph. For $v \in V(G)$, $k$-degree $d_k(v)$ of $v$ is the number of walks of length $k$ of $G$ starting at $v$. In this paper a lower bounds of the spectral radius of $G$ in terms of the $k$-degree of vertices is presented and the upper bounds of energy of a connected graph is obtained.

## 1 Introduction

Let $G = (V, E)$ be a finite graph. For $v \in V(G)$, the degree of $v$ written by $d(v)$, is the number of edges incident with $v$. The number of walks of length $k$ of $G$ starting at $v$ is denoted by $d_k(v)$, is also called $k$-degree of the vertex $v$ and $\dfrac{d_k(v)}{d(v)}$ is called average $k$-degree of the vertex $v$. Clearly, one has $d_0(v) = 1, d_1(v) = d(v)$, and $d_{k+1}(v) = \sum_{w \in N(v)} d_k(w)$, where $N(v)$ is the set of all neighbors of the vertex $v$.

In view of the well-known fact that with $\mathbf{j}$ denote the all one vector defined on the set $V(G)$, the vector $D_k = (d_k(v))_{v \in V}$ coincides with $A^k\mathbf{j}$, where $A = A(G)$ is the adjacency matrix of the graph $G$.

In [3], Dress and Gutman showed an interesting inequality on the number of walks in a graph, and the discussion of the equality holding resulted classification graphs in exactly five classes.

A graph $G$ is called *regular* graph if there exists a constant $r$ such that $d(v) = r$ holds for every $v \in V(G)$, in which case $G$ is also called $r$-regular. Obviously, this is equivalent with the assertion that $A\mathbf{j} = r\mathbf{j}$ holds. Further, a graph $G$ is called *$a, b$-semiregular* if $\{d(v), d(w)\} = \{a, b\}$ holds for all edges $vw \in E(G)$. Clearly, this implies $A^2\mathbf{j} = ab\mathbf{j}$. A semiregular graph that is not regular will henceforth be called *strictly semiregular*. Clearly, a connected strictly semiregular graph must be bipartite.

A graph $G$ is called *harmonic* [3](pseudoregular [13]) if there exists a constants $\mu$ such that $d_2(v) = \mu d(v)$ holds for every $v \in V(G)$ in which case $G$ is also called $\mu$-harmonic, clearly, a graph $G$ is $\mu$-harmonic if and only if $A^2\mathbf{j} = \mu A\mathbf{j}$ holds.( In other words, $A^2\mathbf{j}$ and $A\mathbf{j}$ are linear dependent.)

A graph $G$ is called *semiharmonic* [3] if there exists a constants $\mu$ such that $d_3(v) = \mu d(v)$ holds for every $v \in V(G)$ in which case $G$ is also called $\mu$-semiharmonic, clearly, a graph $G$ is $\mu$-semiharmonic if and only if $A^3\mathbf{j} = \mu A\mathbf{j}$ holds. (In other words, $A^3\mathbf{j}$ and $A\mathbf{j}$ are linear dependent.) Thus every $\mu$-harmonic graph is $\mu^2$-semiharmonic. Also every $a, b$-semiregular graph is $ab$-semiharmonic. A semiharmonic graph that is not harmonic will henceforth be called *strictly semiharmonic.*

Finally, a graph $G$ is called *$(a, b)$-pseudosemiregular* if $\{\frac{d_2(v)}{d(v)}, \frac{d_2(w)}{d(w)}\} = \{a, b\}$ holds for all edges $vw \in E(G)$. A pseudosemiregular graph that is not pseudoregular will henceforth be called *strictly pseudosemiregular.* Clearly, a connected strictly pseudosemiregular graph must be bipartite.

In this paper, we present a lower bound for the spectral radius of a connected graph and give a upper bound for the energy of a graph by using this new lower bound of spectral radius.

## 2 The spectral radius a graph and $k$-degree

Let $G$ be a connected graph. The spectral radius (largest eigenvalue of $A(G)$) of $G$ is denoted by $\rho(G)$. In [4], the following theorem was given:

**Theorem 1** *Let $G$ be a connected graph with degree sequence $d_1, d_2, ..., d_n$. Then*

$$\rho(G) \geq \sqrt{\frac{\sum_{v\in V} d^2(v)}{n}}, \tag{1}$$

*with equality if and only if $G$ is regular or a semiregular.*

In [13], the following theorem was given:

**Theorem 2** *Let $G$ be a connected graph. Then*

$$\rho(G) \geq \sqrt{\frac{\sum_{v\in V} d_2^2(v)}{\sum_{v\in V} d^2(v)}}, \tag{2}$$

*with equality if and only if $G$ is a pseudo-regular graph or a strictly pseudo-semiregular graph.*

In this section we prove a more general result which generalizes and unifies the above two results.

**Lemma 3** *Let $G$ be a connected graph and $k \geq 0$. Then*

$$\rho(G) \geq \sqrt{\frac{\sum_{v\in V} d_{k+1}^2(v)}{\sum_{v\in V} d_k^2(v)}}, \tag{3}$$

*with equality if and only if $A^{k+2}(G)\mathbf{j} = \rho^2(G)A^k(G)\mathbf{j}$.*

**Proof.** Since $D_k^T A^2 D_k = \langle A^{k+1}\mathbf{j}, A^{k+1}\mathbf{j}\rangle = \langle D_{k+1}, D_{k+1}\rangle = \sum_{v\in V} d_{k+1}^2(v)$, thus, by Rayleigh-Ritz Theorem, $\rho(G) = \sqrt{\rho(A^2)} \geq \dfrac{D_k^T A^2 D_k}{\langle D_k, D_k\rangle} \geq \sqrt{\dfrac{\sum_{v\in V} d_{k+1}^2(v)}{\sum_{v\in V} d_k^2(v)}}$, and equality holds if and only if $D_k$ is a eigenvector of $A^2(G)$ corresponding to the eigenvalue $\rho(G)^2$, that is, if and only if $A^{k+2}(G)\mathbf{j} = \rho^2(G)A^k(G)\mathbf{j}$.

For $k = 0$, the above lemma becomes Theorem 1, this is because that $A^2(G)\mathbf{j} = \mu\mathbf{j}$ if and only if $G$ is regular or semiregular (see [3]). By Theorem 1 of [3], every graph $G$ for which some integers $k, l$ with $0 \leq \ l < k$ and some constant $\mu$ such that $d_k(v) = \mu d_l(v)$ for all $v \in V(G)$ (equivalently, $A^k\mathbf{j} = \mu A^l\mathbf{j}$ ) is semiharmonic, and even harmonic in case $k - l$ is odd.) Therefore, for $k \geq 1$, $\rho(G) \geq \sqrt{\dfrac{\sum_{v \in V} d_{k+1}^2(v)}{\sum_{v \in V} d_k^2(v)}}$ and the equality holds if and only if $G$ is a semiharmonic graph. In the next lemma we prove that strictly semiharmonic connected graphs and strictly pseudosemiregular connected graphs are the same.

**Lemma 4** *Let $G$ be a connected graph. Then following are equivalent:*

*(1). $G$ is strictly semiharmonic.*

*(2). $G$ is strictly pseudosemiregular.*

**Proof.** Let $G$ be a strictly semiharmonic graph. Then $G$ must have a vertex $v_0$ of the smallest average 2-degree, say $a = \dfrac{d_2(v_0)}{d(v_0)}$. Let $w_0$ be the vertex that is adjacent to $v_0$ and has the largest average 2-degree among the neighbors of $v_0$, say $b = \dfrac{d_2(w_0)}{d(w_0)}$. Then

$$d_3(w_0) \quad = \sum_{u \in N(v_0)} d_2(u) \geq \frac{d_2(v_0)}{d(v_0)} d_2(w_0) = abd(w_0),$$

with equality holding if and only if all neighbors of $w_0$ have average 2-degree $a$.

$$d_3(v_0) \quad = \sum_{u \in N(w_0)} d_2(u) \leq \frac{d_2(w_0)}{d(w_0)} d_2(v_0) = abd(v_0),$$

with equality holding if and only if all neighbors of $v_0$ have average 2-degree $b$.

Since $G$ is strictly semiharmonic, $a \neq b$ and $d_3(v) = \mu d(v)$ holds for all $v \in V(G)$, all neighbors of $v_0$ must have average 2-degree $b$ and all neighbors of $w_0$ must have average 2-degree $a$. Since $G$ is connected, it follows immediately that $G$ is (bipartite) strictly pseudosemiregular.

If $G$ is strictly pseudosemiregular and let $V = V_1 \cup V_2$ be a bipartition of $V(G)$. Set $a = \dfrac{d_2(u)}{d(u)} (u \in V_1)$ and $b = \dfrac{d_2(v)}{d(v)} (v \in V_2)$ and $a \neq b$. Hence $G$ is not harmonic. For all $u \in V_1$, we have

$$d_3(u) \quad = \sum_{v \in N(u)} d_2(v) = \sum_{v \in N(u)} \frac{d_2(v)}{d(v)} d(v) = bd_2(u) = abd(u)$$

and similarly, $d_3(v) = abd(v)$ for all $v \in V_2$. Thus $d_3(v) = abd(v)$ for all $v \in V$ and hence $G$ is a strictly $ab$-semiharmonic graph.

Combining lemmas 3 and 4 we have the main result which generalizes Theorem 2.

**Theorem 5** *Let $G$ be a connected graph and $k \geq 1$. Then*

$$\rho(G) \geq \sqrt{\frac{\sum_{v\in V} d_{k+1}^2(v)}{\sum_{v\in V} d_k^2(v)}},$$

*with equality if and only if $G$ is pseudoregular or strictly pseudosemiregular.*

**Theorem 6** *Let $G$ be a connected graph and*

$$f(k) = \sqrt{\frac{\sum_{v\in V} d_{k+1}^2(v)}{\sum_{v\in V} d_k^2(v)}}, \quad k \geq 0. \tag{4}$$

*Then $f(k)$ is an increasing sequence and*

$$\lim_{n\to\infty} f(k) = \rho(G).$$

**Proof.** We prove the monotone increasing of $f(k)$ by showing that $f(k+1) \geq f(k)$. Note that the inner product $\langle A^k\mathbf{j}, A^k\mathbf{j}\rangle = (A^k\mathbf{j})^T A^k\mathbf{j} = \sum_{v\in V} d_k^2(v)$.

By Cauchy-Schwarz inequality, we have

$$\langle A^k\mathbf{j}, A^k\mathbf{j}\rangle\langle A^{k+2}\mathbf{j}, A^{k+2}\mathbf{j}\rangle \geq \langle A^k\mathbf{j}, A^{k+2}\mathbf{j}\rangle^2 = \langle A^{k+1}\mathbf{j}, A^{k+1}\mathbf{j}\rangle^2.$$

That is,

$$\frac{\sum_{v\in V} d_{k+2}^2(v)}{\sum_{v\in V} d_{k+1}^2(v)} \geq \frac{\sum_{v\in V} d_{k+1}^2(v)}{\sum_{v\in V} d_k^2(v)}.$$

Hence, $f(k+1) \geq f(k)$ for $k \geq 0$.

Since the sequence $f(k)$ is an monotonically increasing sequence and has a upper bound $\rho(G)$, the limit $\lim_{k\to\infty} f(k)$ must exist. In order to prove the limit it suffices to prove $\lim_{k\to\infty} f(2k) = \rho(G)$.

Let $\rho(G) = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n$ be all eigenvalues of $A(G)$ and $X_1, X_2, \cdots, X_n$ be unit eigenvectors corresponding these eigenvalues of $A(G)$. Then $X_1, X_2, \cdots, X_n$ consist of a orthonormal basis of $\mathcal{R}^n$. Assume that $\mathbf{j} = \sum_{i=1}^n \theta_i X_i$, then $\theta_i = \mathbf{j}^T X_i, i = 1, 2, ..., n$. In order to prove $\lim_{k\to\infty} f(2k) = \rho(G)$ it suffices to prove that $\dfrac{D_{2k}}{\sqrt{\langle D_{2k}, D_{2k}\rangle}}$ approaches a unit eigenvector corresponding the eigenvalue $\rho^2(G)$ of $A^2(G)$ when $k \to \infty$. Note that $\dfrac{D_{2k}}{\sqrt{\langle D_{2k}, D_{2k}\rangle}} = \dfrac{A^{2k}\mathbf{j}}{\sqrt{\langle A^{2k}\mathbf{j}, A^{2k}\mathbf{j}\rangle}} = \dfrac{A^{2k}\mathbf{j}}{\sum_{v\in V} d_{2k}^2(v)}$ and

$$A^{2k}\mathbf{j} = A^{2k}\sum_{i=1}^n \theta_i X_i = \sum_{i=1}^n \theta_i \lambda_i^{2k} X_i,$$

we have

$$\sum_{v \in V} d_{2k}^2(v) = \sum_{i=1}^{n} \theta_i^2 \lambda_i^{4k}.$$

If $G$ is nonbipartite, since $\theta_1 > 0$ and $\lambda_1 > |\lambda_i|$ for all $i = 2, 3, ..., n$, then the vector $\frac{\theta_i \lambda_i^{2k} X_i}{\sqrt{\sum_{i=1}^{n} \theta_i^2 \lambda_i^{4k}}}$ approaches $X_1$ if $i = 1$, 0 if $i > 1$. Thus the eigenvector $\frac{D_{2k}}{\sqrt{\langle D_{2k}, D_{2k} \rangle}}$ approaches $X_1$ and the result follows.

If $G$ is bipartite, since $\theta_1 > 0$ and $\lambda_1 > |\lambda_i|$ for all $i = 2, 3, ..., n-1$, $\lambda_n = -\lambda_1$, then the vector $\frac{\theta_i \lambda_i^{2k} X_i}{\sqrt{\sum_{i=1}^{n} \theta_i^2 \lambda_i^{4k}}}$ approaches $\frac{\theta_1 X_1}{\sqrt{\theta_1^2 + \theta_n^2}}$ if $i = 1$, 0 if $1 < i < n$, $\frac{\theta_n X_n}{\sqrt{\theta_1^2 + \theta_n^2}}$ if $i = n$. Thus the eigenvector $\frac{D_{2k}}{\sqrt{\langle D_{2k}, D_{2k} \rangle}}$ approaches $\frac{\theta_1 X_1 + \theta_n X_n}{\sqrt{\theta_1^2 + \theta_n^2}}$, which is a unit eigenvector corresponding the eigenvalue $\rho^2(G)$ of $A^2(G)$ and the result follows.

## 3 Upper bounds for the energy of a graph

The *energy* of a graph $G$, denoted by $E(G)$, is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$, where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of the adjacency matrix of $G$. This concept was introduced by I. Gutman and is studied intensively in mathematical chemistry, since it can be used to approximate the total $\pi$-electron energy of a molecule(see [5] ). In 1971 McClelland discovered the first upper bound for $E(G)$ as follows:

$$E(G) \leq \sqrt{2mn}. \tag{5}$$

Since then, numerous other bounds for $E(G)$ were found (see [1,2,6–10,12,14–16]). Recently, Yu et. al [14] proved the following result:

**Theorem 7** *Let $G$ be a nonempty graph with $n$ vertices and $m$ edges. Then*

$$E(G) \leq \sqrt{\frac{\sum_{v \in V(G)} d_2^2(v)}{\sum_{v \in V(G)} d^2(v)}} + \sqrt{(n-1)\left(2m - \frac{\sum_{v \in V(G)} d_2^2(v)}{\sum_{v \in V(G)} d^2(v)}\right)}. \tag{6}$$

*Equality holds if and only if one of the following statements holds:*

*(1) $G \cong \frac{n}{2} K_2$;*

*(2) $G \cong K_n$;*

*(3) $G$ is a non-bipartite connected $\mu$-pseudoregular graph with three distinct eigenvalues $\mu, \sqrt{\frac{2m-\mu^2}{n-1}}, -\sqrt{\frac{2m-\mu^2}{n-1}}$, where $\mu > \sqrt{\frac{2m}{n}}$.*

*Remark* In fact, the graph appears in (3) of above Theorem must be non-completed strongly regular graph with two nontrivial eigenvalues both with absolute value $\sqrt{\frac{2m-(\frac{2m}{n})^2}{n-1}}$, for details see the proof of the next Theorem.

The following is the main results of this section which generalize the above result. Since general case is not substantially different, we concentrate on the particular case of connected graph for the sake of readability.

**Theorem 8** *Let $G$ be a connected graph with $n(n \geq 2)$ vertices and $m$ edges. Then*

$$E(G) \leq \sqrt{\frac{\sum_{v\in V(G)} d_{k+1}^2(v)}{\sum_{v\in V(G)} d_k^2(v)}} + \sqrt{(n-1)\left(2m - \frac{\sum_{v\in V(G)} d_{k+1}^2(v)}{\sum_{v\in V(G)} d_k^2(v)}\right)}\,. \tag{7}$$

*Equality holds if and only if $G$ is the complete graph $K_n$ or $G$ is a strongly regular graph with two nontrivial eigenvalues both with absolute value $\sqrt{\frac{2m-(\frac{2m}{n})^2}{n-1}}$.*

**Proof.** Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of $G$. By the Cauchy-Scharz inequality we have

$$\begin{aligned} E(G) &= \sum_{i=1}^{n} |\lambda_i| = \lambda_1 + \sum_{i=2}^{n} |\lambda_i| \\ &\leq \sqrt{(n-1)\sum_{i=2}^{n} \lambda_i^2} = \sqrt{(n-1)(2m-\lambda_1^2)}\,. \end{aligned}$$

Now since the function $F(x) = x + \sqrt{(n-1)(2m-x^2)}$ decreases on the interval $\sqrt{2m/n} \leq x \leq \sqrt{2m}$. By Theorem 6 we have

$$\lambda_1 \geq f(k) \geq f(0) = \sqrt{\frac{\sum_{v\in V(G)} d^2(v)}{n}} \geq \sqrt{\frac{2m}{n}}.$$

Hence $F(\lambda_1) \leq F(\sqrt{\sum_{v\in V(G)} d_{k+1}(v)^2/d_k(v)^2}\ )$ and

$$E(G) \leq \sqrt{\frac{\sum_{v\in V(G)} d_{k+1}^2(v)}{\sum_{v\in V(G)} d_k^2(v)}} + \sqrt{(n-1)\left(2m - \frac{\sum_{v\in V(G)} d_{k+1}^2(v)}{\sum_{v\in V(G)} d_k^2(v)}\right)}\,. \tag{8}$$

If the connected graph $G$ is a complete graph $K_n$ or a strong regular graph with two non-trivial eigenvalues both with absolute values $\sqrt{\frac{2m-(\frac{2m}{n})^2}{n-1}}$ then it is easy to check that the equality holds.

Conversely, if the equality holds, according the above proof, we have

$$\lambda_1 = \sqrt{\frac{\sum_{v\in V(G)} d_{k+1}^2}{\sum_{v\in V(G)} d_k^2}},$$

which implies that $G$ is pseudo-semiregular and $|\lambda_i| = \sqrt{\dfrac{2m-\lambda_1^2}{n-1}}$ for $i = 2, 3, ..., n$. Note that a graph has only one distinct eigenvalue if and only if it has no edges and a graph has two distinct eigenvalues if and only if it is a complete graph. Since $G$ is connected, we reduced to the following two cases:

(1) $G$ has two distinct eigenvalues. In this case $G \cong K_n$.

(2) $G$ has three distinct eigenvalues. In this case, $\lambda_1 = \sqrt{\dfrac{\sum_{v\in V(G)} d_{k+1}^2}{\sum_{v\in V(G)} d_k^2}}$ and $|\lambda_i| = \sqrt{\dfrac{2m-\lambda_1^2}{n-1}}$ for $i = 2, 3, ..., n$. Since $G$ is connected, $\lambda_1 > \lambda_i$, $\lambda_i \neq 0$ for $i = 2, ..., n$. Thus $G$ must be regular (else $G$ has 0 as an eigenvalue) and non-bipartite ( else $G$ has least four distinct eigenvalues). Hence $G$ is $\lambda_1$-regular ($\lambda_1 = \dfrac{2m}{n}$) and has exact three distinct eigenvalues. Thus $G$ is strong regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\dfrac{\left(2m - (\frac{2m}{n})^2\right)}{n-1}}$.

Similarly, (similar to [7, 14, 15]) we may prove

**Theorem 9** *Let $G$ be a connected bipartite graph with $n (n \geq 2)$ vertices and $m$ edges. Then*

$$E(G) \leq 2\sqrt{\frac{\sum_{v\in V(G)} d_{k+1}^2(v)}{\sum_{v\in V(G)} d_k^2(v)}} + \sqrt{(n-2)\left(2m - 2\frac{\sum_{v\in V(G)} d_{k+1}^2(v)}{\sum_{v\in V(G)} d_k^2(v)}\right)}. \qquad (9)$$

*Equality holds if and only if $G$ is the complete bipartite graph or $G$ is the incidence graph of a symmetric 2-$(\nu, k, \lambda)$-design with $k = \dfrac{2m}{n}, n = 2\nu$ and $\lambda = \dfrac{k(k-1)}{\nu - 1}$.*

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