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New Upper Bounds for the Hückel Energy of Graphs

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Abstract

Let $G = (V, E)$ be a graph on n vertices, and let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be eigenvalues of G. The Hückel energy of G, $HE(G)$, is defined as

$$HE(G) = \begin{cases} 2\sum\limits_{i=1}^{r} \lambda_i, & if\ n = 2r \\ 2\sum\limits_{i=1}^{r} \lambda_i + \lambda_{r+1}, & if\ n = 2r + 1\ . \end{cases}$$

In this paper, we present some new upper bounds for $HE(G)$, from which we can improve some known results.

1. Introduction

All graphs considered here are finite, undirected and simple. Undefined terminology and notation may refer to [1]. Let $G = (V(G), E(G))$ be a graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $|E(G)| = m$. For $v_i \in V(G)$, the *degree* of v_i, written by $d(v_i)$ or d_i,

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is the number of edges incident with v_i. The number of walks of length k starting at v_i is called *k-degree* of the vertex v_i and is denoted by $d_{k,i}$. The quantity $\frac{d_{k,i}}{d_i}$ is called *average k-degree* of v_i. Clearly, one has $d_{0,1} = 1$, $d_{1,i} = d_i$, and $d_{k+1,i} = \sum_{v_j \in N(v_i)} d_{k,j}$, where $N(v_i)$ is the set of all neighbors of the vertex v_i.

A graph G is called *k-regular* (or resp., *k-pseudo-regular*, see [4]) if there exists a constant k such that $d_i = k$ (or resp., $\frac{d_{2,i}}{d_i} = k$) holds for $i = 1, 2, \ldots, n$. Further, a graph G is called *k, l-semi-regular* (or resp., *k, l-pseudo-semi-regular*) if $\{d_i, d_j\} = \{k, l\}$ (or resp., $\{\frac{d_{2,i}}{d_i}, \frac{d_{2,j}}{d_j}\} = \{k, l\}$) holds for all the edges $v_iv_j \in E(G)$. A semi-regular graph (or resp., pseudo-semi-regular graph) that is not regular (or resp., pseudo-regular) will henceforth be called *strictly semi-regular* (or resp., *strictly pseudo-semi-regular*).

Let $A = A(G)$ be the adjacency matrix of a graph G, and let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of A. The *energy* of G, denoted by $E(G)$, is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$, which gives a good approximation for the total π-electron energy of a molecule whose molecular graph is G (see [8–10, 17]). The *Hückel energy* of G, denoted by $HE(G)$, is defined as

$$HE(G) = \begin{cases} 2\sum_{i=1}^{r} \lambda_i, & if\ n = 2r \\ 2\sum_{i=1}^{r} \lambda_i + \lambda_{r+1}, & if\ n = 2r+1\ . \end{cases}$$

The concept of Hückel energy was first introduced by Hückel [12] in 1931, and explicitly used in 1940 by Coulson [2]. In comparison with the energy of a graph the Hückel energy of a graph gives a better approximation for the total π-electron energy of a conjugated molecule (see, e. g., [5]). Clearly for any graph G, $HE(G) \leq E(G)$, and if G is bipartite (which is the case with the vast majority of molecular graphs [9,13,14,18]), then equality holds. Obviously, all upper bounds for the energy (see [11,15,16,19,20]) also give upper bounds for the Hückel energy of graphs. In [6], Ghorbani, Koolen, and Yang presented the following upper bounds for $HE(G)$:

$$HE(G) \leq \begin{cases} \dfrac{2m}{n-1} + \dfrac{\sqrt{2m(n-2)(n^2-n-2m)}}{n-1} & if\ m \leq \dfrac{n^3}{2(n+2)} \\ \dfrac{2}{n}\sqrt{mn(n^2-2m)} < \dfrac{4m}{n} & otherwise \end{cases} \tag{1}$$

if n is even, and

$$HE(G) \leq \begin{cases} \dfrac{2m}{n-1} + \dfrac{\sqrt{2mn(n^2-3n+1)(n^2-n-2m)}}{n(n-1)} & if\ m \leq \dfrac{n^2(n-3)^2}{2(n^2-4n+11)} \\ \dfrac{1}{n}\sqrt{2m(2n-1)(n^2-2m)} & otherwise \end{cases} \tag{2}$$

if n is odd.

In this paper, we obtain some new upper bounds for $HE(G)$ of a graph G in terms of n, m, and $d_{k,i}$, from which we can improve some known results.

2. Preliminaries

In order to obtain the sharp upper bounds for the Hückel energy of a graph, we need the following lemmas.

In [11], for a connected graph G, Hou, Tang and Woo obtained an upper bound of $\lambda_1(G)$. In fact, it also holds for any nonempty graph.

Lemma 2.1 [11]. *Let G be a non-empty graph of order n and*

$$f(k) = \sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} \quad , \quad k \geq 0 \ .$$

Then $f(k)$ is an increasing sequence and $\lambda_1 \geq f(k)$ with equality for $k \geq 1$ if and only if G is pseudo-regular or strictly pseudo-semi-regular.

Lemma 2.2 [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 2.3 [6]. *Let G be a graph with n vertices and m edges. Suppose $r := \lfloor n/2 \rfloor$, and $\alpha := \sum\limits_{i=1}^{r} \lambda_i^2$. For $m \geq n-1 \geq 2$, we have*

$$\frac{m}{r} \geq \sqrt{\frac{\alpha}{r}}\ .$$

Lemma 2.4 [6]. *Let G be a graph with n vertices and m edges where n is odd. Suppose $r := \lfloor n/2 \rfloor$, $\alpha := \sum\limits_{i=1}^{r} \lambda_i^2$, and $\beta := \lambda_{r+1}$. For $m \geq n-1 \geq 4$, we have $2m - \alpha \geq (r+1)\beta^2$.*

3 The Hückel Energy of Graphs

In this section, we will present some new upper bounds for $HE(G)$ of a graph G in terms of n, m, and $d_{k,i}$ according to the parity of n, respectively.

3.1 The Upper Bound for Even Order Graphs

In this subsection, we give an upper bound for $HE(G)$ of an even order graph G and characterize those graphs for which this bound is best possible. Denote

$$M_e = \frac{(n+2)\sum\limits_{i=1}^{n} d_{k+1,i}^2}{2n\sum\limits_{i=1}^{n} d_{k,i}^2}\ .$$

Theorem 3.1. *Let G be a graph on $n = 2r$ vertices and m edges, where $r \geq 2$. Then*

$$HE(G) \leq \begin{cases} \dfrac{n}{n-1}\left(\sqrt{\dfrac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}} + \sqrt{(n-2)\left(\dfrac{2m(n-1)}{n} - \dfrac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}\right)}\right) & if\ m \geq M_e \\ \sqrt{2n\left(2m - \dfrac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}\right)} & otherwise. \end{cases} \tag{3}$$

Proof. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of G, then $\sum\limits_{i=1}^{n} \lambda_i = 0$ and $\sum\limits_{i=1}^{n} \lambda_i^2 = 2m$. Let $\alpha = \sum\limits_{i=1}^{r} \lambda_i^2$, then $2m - \alpha = \sum\limits_{i=r+1}^{n} \lambda_i^2$. By the Cauchy–Schwarz inequality,

$$HE(G) = 2\sum_{i=1}^{r} \lambda_i \leq 2\lambda_1 + 2\sqrt{(r-1)(\alpha - \lambda_1^2)}\ .$$

The function $x \mapsto x + \sqrt{(r-1)(\alpha - x^2)}$ decreases on the interval $\sqrt{\frac{\alpha}{r}} \leq x \leq \sqrt{\alpha}$. From Lemma 2.3, we have $\frac{m}{r} \geq \sqrt{\frac{\alpha}{r}}$. By Lemma 2.1, we have

$$\sqrt{\frac{\alpha}{r}} \ \leq \ \frac{m}{r} = \frac{2m}{n} \leq \sqrt{\frac{\sum\limits_{i=1}^{n} d_i^2}{n}} = f(0) \leq f(k) \leq \lambda_1 \tag{$*$}$$

thus

$$HE(G) \leq f_1(\alpha) := 2\sqrt{\frac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}} + 2\sqrt{(r-1)\left(\alpha - \frac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}\right)}.$$

On the other hand,

$$HE(G) = -2\sum_{i=r+1}^{n} \lambda_i \leq 2\sqrt{r\left(\sum_{i=r+1}^{n} \lambda_i^2\right)} \leq f_2(\alpha) := 2\sqrt{r(2m-\alpha)}\ .$$

Let $f(\alpha) := \min\{f_1(\alpha), f_2(\alpha)\}$. We determine the maximum of f. Note that f_1 and f_2 are increasing and decreasing function in α, respectively. Therefore, $\max f = f(\alpha_0)$

where α_0 is the unique point with $f_1(\alpha_0) = f_2(\alpha_0)$. So in the following, we find the solution of equation $f_1(\alpha) = f_2(\alpha)$. To do so, let

$$\sigma = \sqrt{\alpha - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}}$$

and consider the equation

$$\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} + \sqrt{(r-1)}\sigma = \sqrt{r\left(2m - \sigma^2 - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}.$$

This equation has the roots

$$\sigma_{1,2} = -\frac{1}{2r-1}\left(\sqrt{\frac{(r-1)\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} \mp \sqrt{2r\left(2mr - m - \frac{r\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}\right).$$

If $m \geq M_e$, i. e.,

$$m \geq \frac{(r+1)\sum_{i=1}^{n} d_{k+1,i}^2}{2r\sum_{i=1}^{n} d_{k,i}^2}$$

then $\sigma_1 \geq 0$ and so

$$\begin{aligned} HE(G) &\leq 2\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} + 2\sqrt{r-1}\sigma_1 \\ &= \frac{n}{n-1}\left(\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} + \sqrt{(n-2)\left(\frac{2m(n-1)}{n} - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}\right). \qquad (4) \end{aligned}$$

Otherwise, $f_1(\alpha) > f_2(\alpha)$, then $f(\alpha) = f_2(\alpha)$. Hence, for $m < M_e$,

$$HE(G) \leq 2\sqrt{r\left(2m - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)} = \sqrt{2n\left(2m - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}. \tag{5}$$

This complete the proof of theorem 3.1. ∎

Remark 3.2. Here we show that the equality in (4) holds if and only if $G \cong \frac{n}{2}K_2$ or G is a strongly regular graph with parameters $(n, k, \lambda, \mu) = (4t^2+4t+2, 2t^2+3t+1, t^2+2t, t^2+2t+1)$ for some positive integer t and no graph can attain the upper bond in (5). Let us keep the notation of the proof of Theorem 3.1. If $G \cong \frac{n}{2}K_2$ or G is a strongly regular graph with parameters $(n, k, \lambda, \mu) = (4t^2+4t+2, 2t^2+3t+1, t^2+2t, t^2+2t+1)$, it is easy to check that the equality (4) holds. Conversely, if the equality (4) holds. Let $m \geq M_e$. Then

1. $\lambda_1 = \sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}}$
2. $\lambda_2 = \lambda_3 = \cdots = \lambda_r = \frac{\sigma_1}{\sqrt{r-1}}$
3. $\lambda_{r+1} = \lambda_{r+2} = \cdots = \lambda_n = -\frac{1}{\sqrt{r}}\sqrt{2m - \sigma_1^2 - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}}$.

Note that G at least has two distinct eigenvalues, we are reduced to the following two possibilities:

(i) G has two distinct eigenvalues.

If G has only two distinct eigenvalues, then $\lambda_1 = \lambda_2 = \cdots = \lambda_r$. Since $\lambda_{r+1} = \lambda_{r+2} = \cdots = \lambda_n$, $\sum_{i=1}^{n} \lambda_i = 0$ and $\sum_{i=1}^{n} \lambda_i^2 = 2m$, we have $\lambda_1 = \lambda_2 = \cdots = \lambda_r = \sqrt{2m/n}$ and $\lambda_{r+1} = \lambda_{r+2} = \cdots = \lambda_n = -\sqrt{2m/n}$. By Lemma 2.2, $\sqrt{2m/n} = 1$. Hence $2m = n$, which implies $G \cong \frac{n}{2}K_2$.

(ii) G has three distinct eigenvalues.

Since $\lambda_1 > \lambda_i$, $\lambda_i \neq 0$ for $i = 2, 3, \ldots, n$, G must be regular (else G has 0 as an eigenvalue) and non-bipartite (else G at least has four distinct eigenvalues). Hence G is λ_1-regular ($\lambda_1 = 2m/n$) and has three distinct eigenvalues. From [Lemma 10.2.1 in [7]], we have G is a strongly regular graph. From [Lemma 10.3.5 in [7]], we have G is a strongly regular graph with parameters $(n, k, \lambda, \mu) = (4t^2+4t+2, 2t^2+3t+1, t^2+2t, t^2+2t+1)$.

If $m < M_e$, then the equality (5) holds if and only if

1. $\lambda_1 = \sqrt{\dfrac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}}$

2. $\lambda_2 = \lambda_3 = \cdots = \lambda_r = 0$

3. $\lambda_{r+1} = \lambda_{r+2} = \cdots = \lambda_n = -\dfrac{1}{\sqrt{r}}\sqrt{2m - \dfrac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}}$.

The first condition shows that G is pseudo-semi-regular. Since G is a graph with only one positive eigenvalue. Then from [Theorem 6.7 in [3]], G is a complete multipartite graph. As the rank of a complete multipartite graph equals the number of its parts, G must have $r+1$ parts. Such a graph can not be pseudo-semi-regular, then no graph can attain the bound in (5).

3.2 The Upper Bound for Odd Order Graphs

In this subsection, we give an upper bound for $HE(G)$ of an odd order graph G and discuss the equality case. Denote

$$M_o = \frac{(n^2 - 4n + 11)\sum\limits_{i=1}^{n} d_{k+1,i}^2}{2(n^2 - 6n + 9)\sum\limits_{i=1}^{n} d_{k,i}^2} .$$

Theorem 3.3. *Let G be a graph with $n = 2r+1$ vertices and m edges, where $r \geq 2$. Then*

$$HE(G) \leq \begin{cases} \dfrac{n}{n-1}\left(\sqrt{\dfrac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}} + \sqrt{\dfrac{n^2-3n+1}{n}\left(\dfrac{2m(n-1)}{n} - \dfrac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}\right)}\right) & if\ m \geq M_o \\ \sqrt{(2n-1)\left(2m - \dfrac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}\right)} & otherwise. \end{cases} \tag{6}$$

Proof. Let $\alpha = \sum\limits_{i=1}^{r} \lambda_i^2$, $\beta = \lambda_{r+1}$. From Lemma 2.4, we have $2m - \alpha \geq (r+1)\beta^2$. By the Cauchy–Schwarz inequality, we have

$$HE(G) = 2\sum_{i=1}^{r} \lambda_i + \lambda_{r+1} \leq 2\lambda_1 + 2\sqrt{(r-1)(\alpha - \lambda_1^2)} + \beta\ .$$

The function $x \mapsto 2x + 2\sqrt{(r-1)(\alpha - x^2)} + \beta$ decreases on the interval $\sqrt{\frac{\alpha}{r}} \leq x \leq \sqrt{\alpha}$. Since

$$\sqrt{\frac{\alpha}{r}} \leq \sqrt{\frac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}} \leq \lambda_1$$

then

$$HE(G) \leq f_1(\alpha,\beta) := 2\sqrt{\frac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}} + 2\sqrt{(r-1)\left(\alpha - \frac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}\right)} + \beta\ .$$

In a similar manner as the proof of Theorem 3.1, we have

$$HE(G) \leq f_2(\alpha,\beta) := 2\sqrt{r(2m - \alpha - \beta^2)} - \beta\ .$$

Let

$$f(\alpha,\beta) := \min\{f_1(\alpha,\beta), f_2(\alpha,\beta)\}\,.$$

We determine the maximum of f over the compact set

$$D := \left\{ (\alpha,\beta) \ : \ \alpha \geq \frac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}, \quad 2m-(r+1)\beta^2 \geq \alpha \right\}.$$

Note that for $(\alpha,\beta) \in D$ one has $-\beta_0 \leq \beta \leq \beta_0$, where

$$\beta_0 = \sqrt{\frac{2}{n+1}\left(2m - \frac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}\right)}.$$

Neither the gradient of f_1 nor that of f_2 has a zero in interior of D. So the maximum of f occurs in the set

$$L = \{(\alpha,\beta) : f_1(\alpha,\beta) = f_2(\alpha,\beta)\}$$

where the gradient of f does not exist or it occurs in the boundary of D consisting of

$$D_1 = \left\{ (\alpha,\beta) : \alpha = \frac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}, -\beta_0 \leq \beta \leq \beta_0 \right\}$$

$$D_2 = \left\{ (\alpha,\beta) : \alpha = 2m-(r+1)\beta^2, -\beta_0 \leq \beta \leq \beta_0 \right\}.$$

First we examine max $f_{|L}$. Let

$$p = \sqrt{\frac{\sum\limits_{i=1}^{n} d_{k+1,i}^2}{\sum\limits_{i=1}^{n} d_{k,i}^2}} \quad \text{and} \quad \sigma = \sqrt{\alpha - p^2}\ .$$

In order to determine (α,β) satisfying $f_1(\alpha,\beta) = f_2(\alpha,\beta)$, it is enough to find the zeros of the following quadratic form:

$$2(n-2)\sigma^2 + 2\sqrt{2(n-3)}(p+\beta)\sigma + (n+1)(p^2+\beta^2) + 4p\beta - 2m(n-1) = 0\ .$$

The zeros are

$$\sigma_{1,2} = \frac{-\sqrt{2(n-3)}(p+\beta) \pm \sqrt{(n-1)[4(n-2)m - 4p\beta - 2(n-1)(p^2+\beta^2)]}}{2(n-2)} \, .$$

Note that $\sigma_2 < 0$ and so is not feasible. Let $h(\beta) = (n+1)(p^2+\beta^2) + 4p\beta - 2m(n-1)$. Then $\sigma_1 \geq 0$ if and only if $h(\beta) \leq 0$. Moreover $h(\beta) \leq h(\beta_0)$.

If $m \geq M_o$, i. e.,

$$m \geq \frac{(n^2-4n+11)\sum_{i=1}^{n} d_{k+1,i}^2}{2(n^2-6n+9)\sum_{i=1}^{n} d_{k,i}^2}$$

then we have $h(\beta_0) \leq 0$ and $\sigma_1 \geq 0$. Thus, with this condition on m, $f_1(\alpha, \beta)$ becomes

$$f_1(\sigma_1, \beta) := 2\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} + 2\sqrt{r-1}\sigma_1 + \beta$$

where $f_1(\sigma_1, \beta)$ is a function of β. If $f_1'(\sigma_1, \beta) \geq 0$, we have

$$(n-1)(n^2-3n+1)\beta^2 + 2(n^2-3n+1)\beta\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} + (n-1)\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2} - 2m \leq 0 \, .$$

The roots of $f_1'(\sigma_1, \beta) = 0$ are

$$\beta_{1,2} = -\frac{1}{n-1}\left(\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} \mp \sqrt{\frac{1}{n^2-3n+1}\left(2m(n-1) - \frac{n\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}\right) .$$

Note that if $\beta_2 \leq \beta \leq \beta_1$, then $f_1'(\sigma_1, \beta) \geq 0$; if $\beta \geq \beta_1$ or $\beta \leq \beta_2$, then $f_1'(\sigma_1, \beta) \leq 0$. Since $f_1'(\sigma_1, \beta_0) \geq 0$ and $f_1'(\sigma_1, -\beta_0) \geq 0$, we have $-\beta_0 \leq \beta_2 \leq \beta_1 \leq \beta_0$. Moreover, $\beta_1 \leq 0$. Note that $f_1(\sigma_1, \beta)$ decreases for $\beta_1 \leq \beta \leq \beta_0$, and $-\beta_0 \leq \beta \leq \beta_1$; increases for $\beta_2 \leq \beta \leq \beta_1$. In order to find $\max f_1(\sigma_1, \beta)$, we only need compare $f_1(\sigma_1, \beta_1)$ and

$f_1(\sigma_1, -\beta_0)$. It is easily seen that $f_1(\sigma_1, \beta_0) \geq f_1(\sigma_1, -\beta_0)$, then $f_1(\sigma_1, \beta_1) \geq f_1(\sigma_1, -\beta_0)$. Therefore, $f_{|L} = f_1(\sigma_1, \beta_1)$. Thus for $m \geq M_o$, we have

$$\max f_{|L} = \frac{n}{n-1}\left(\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} + \sqrt{(n^2-3n+1)\left(\frac{2m(n-1)}{n^2} - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{n\sum_{i=1}^{n} d_{k,i}^2}\right)}\right). \tag{7}$$

Otherwise, $\sigma_1 < 0$, and $f_1(\alpha, \beta) > f_2(\alpha, \beta)$, then $f(\alpha, \beta) = f_2(\alpha, \beta)$. We have for any $(\alpha, \beta) \in D$,

$$f_2(\alpha, \beta) \leq f_2\left(\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}, \beta\right).$$

It is easily seen that the maximum of f_2 occurs at

$$\beta_3 = -\sqrt{\frac{1}{2n-1}\left(2m - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}.$$

Therefore,

$$\max f_2 = f_2\left(\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}, \beta_3\right) = \sqrt{(2n-1)\left(2m - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}.$$

Thus for $m < M_o$, we have

$$HE(G) \leq \sqrt{(2n-1)\left(2m - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}. \tag{8}$$

In the rest of proof, we determine $\max f$ for $m \geq M_o$.

On D_1, we have

$$\max f_{|D_1} \leq f_1\left(\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}, \beta_0\right) = 2\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} + \sqrt{\frac{2}{n+1}\left(2m - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}. \tag{9}$$

On D_2, one has

$$f_1(\beta) = 2\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} + 2\sqrt{(r-1)\left(2m - (r+1)\beta^2 - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)} + \beta$$

$$f_2(\beta) = (n-1)|\beta| - \beta\,.$$

In order to find $\max f_{|D_2}$, we look for the points where $f_1(\beta) = f_2(\beta)$.

For $\beta \leq 0$, if $f_1(\beta) \leq f_2(\beta)$, we have

$$2(n^2-1)\beta^2 + 4(n+1)\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}}\beta + \frac{2(n-1)\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2} - 4(n-3)m \geq 0\ .$$

The solution of $f_1(\beta) = f_2(\beta)$ is

$$\beta_{4,5} = -\frac{1}{n-1}\left(\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} \mp \sqrt{\frac{n-3}{n+1}\left(2m(n-1) - \frac{n\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}\right).$$

If $f_1(\beta) \leq f_2(\beta)$, then $\beta \geq \beta_4$ or $\beta \leq \beta_5$. Since $f_1(-\beta_0) \leq f_2(-\beta_0)$, we have $-\beta_0 \leq \beta_5$. It is seen that $f_2(\beta_4) \leq f_2(\beta_5)$.

For $\beta \geq 0$, if $f_1(\beta) \leq f_2(\beta)$, we have

$$2(n^2-4n+3)\beta^2 - 4(n-3)\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}}\beta + \frac{2(n-1)\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2} - 4(n-3)m \geq 0\ .$$

The solution of $f_1(\beta) = f_2(\beta)$ is

$$\beta_{6,7} = \frac{1}{n-1}\left(\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} \pm \sqrt{\frac{1}{n-3}\left(2m(n^2-4n+3) - (n^2-3n+4)\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}\right).$$

If $f_1(\beta) \leq f_2(\beta)$, then $\beta \geq \beta_6$ or $\beta \leq \beta_7$. Since $f_1(\beta_0) \leq f_2(\beta_0)$, we have $\beta_0 \geq \beta_6$. It is seen that $f_2(\beta_6) \geq f_2(\beta_7)$. Moreover $f_2(\beta_5) > f_2(\beta_6)$ (we can easily show that $-n\beta_5 \geq (n-2)\beta_6$). Therefore $\max f_{|D_2} = f_2(\beta_5)$. Thus for $m \geq M_o$, we have

$$\max f_{|D_2} = \tfrac{n}{n-1}\left(\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} + \sqrt{\tfrac{n-3}{n+1}\left(2m(n-1) - \frac{n\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}\right). \tag{10}$$

Comparing (7), (9), and (10), for $m \geq M_o$, we get

$$HE(G) \leq \frac{n}{n-1}\left(\sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} + \sqrt{\frac{n^2-3n+1}{n}\left(\frac{2m(n-1)}{n} - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}\right)}\right). \tag{11}$$

This complete the proof of theorem 3.3. ■

Remark 3.4. Here we show that no graph can attain the bound in (8) and (11). Let us keep the notation of the proof of Theorem 3.3. First let $m \geq M_o$. Then

1. $\lambda_1 = \sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}}$
2. $\lambda_2 = \lambda_3 = \cdots = \lambda_r = \frac{\sigma_1}{\sqrt{r-1}}$
3. $\lambda_{r+1} = \beta_5$
4. $\lambda_{r+2} = \lambda_{r+3} = \cdots = \lambda_n = -\frac{1}{\sqrt{r}}\sqrt{2m - \beta_5^2 - \sigma_1^2 - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}}$.

Since $\lambda_1 > \lambda_i$, $\lambda_i \neq 0$ for $i = 2, 3, \ldots, n$, G must be regular ($\lambda_1 = 2m/n$). Since $\lambda_{r+1} = \beta_5 < 0$, by a similar argument as [Remark 6 in [6]], we have no graph can attain the upper bond in (11).

If $m < M_o$, then the equality holds if and only if

$$\lambda_1 = \sqrt{\frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}}$$

$$\lambda_2 = \cdots = \lambda_r = 0 \quad ; \quad \lambda_{r+1} = \beta_3$$

and

$$\lambda_{r+2} = \cdots = \lambda_n = -\frac{1}{\sqrt{r}} \sqrt{2m - \beta_3^2 - \frac{\sum_{i=1}^{n} d_{k+1,i}^2}{\sum_{i=1}^{n} d_{k,i}^2}} \; .$$

By a similar argument as Remark 3.2, we have no graph can attain the upper bond in (8).

Note 3.5. By (∗), the bounds (3) and (6) are better than (1) and (2), respectively.

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