Validity of Akbari's Energy Conjecture for Threshold Graphs[1]

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Abstract

Let G be a graph of order n, and let $\Delta(G)$, $\delta(G)$ and $\bar{d}$ be the maximum, minimum and average degrees of G, respectively. In 2020, Akbari and Hosseinzadeh proposed a conjecture that $\mathcal{E}(G) \geq \Delta(G) + \delta(G)$ for all non-singular graphs G. Recently, they gave a strengthened version claiming that $\mathcal{E}(G) \geq n - 1 + \bar{d}$ for all non-singular graphs G, except two counterexamples of order 4. They proved this new conjecture for regular graphs, bipartite graphs, planar graphs and graphs with some other special properties. In this paper, we continue the study of the conjecture and find that it is true for the family of threshold graphs of order at least 5.

Keywords:Graph energy; non-singular graph; threshold graph

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1 Introduction

Throughout this paper, all graphs are simple, finite and undirected. Let G be a graph. We denote the vertex set and the edge set of G by $V(G)$ and $E(G)$, respectively. We write $|V(G)| = n$ and $|E(G)| = m$ unless otherwise stated, and call them the *order* and the *size* of G, respectively. The maximum, the minimum and the average degree of G is denoted by $\Delta(G)$, $\delta(G)$, and $\bar{d}$, respectively.

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Let $A(G)$ be the adjacency matrix of a graph G of order n, and denote the eigenvalues of $A(G)$ by $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. G is said to be *singular* if $A(G)$ is a singular matrix, i.e., $det(A(G)) = 0$. The *energy* of a graph G, denoted by $\mathcal{E}(G)$, is defined as $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$. In 1978, Gutman [13] firstly introduced the concept of the energy for graphs, on the basis of The total π-electron energy in a conjugated hydrocarbon. For more knowledge on graph energy, we refer the reader to [16].

Bounds of graph energy have been variously studied. In 2020, Akbari and Hosseinzadeh [6] found a lower bound using the fact that if $x > 0$, then $x > \ln x + 1$. From this inequality, it follows that

$$\begin{aligned}\mathcal{E}(G) =& \lambda_1 + \sum_{i=2}^{n} |\lambda_i| \geq n - 1 + \lambda_1 + \ln |\lambda_2 \cdots \lambda_n| \\ &= n - 1 + \lambda_1 + \ln |\det(A(G))| - \ln \lambda_1.\end{aligned}$$

Since $n - 1 \geq \Delta(G)$ and $\lambda_1 \geq \delta(G)$, they proposed the following conjecture.

Conjecture 1.1. *The energy of a non-singular graph G satisfies the following inequality*

$$\mathcal{E}(G) \geq \Delta(G) + \delta(G).$$

Although the conjecture remains open, there have been some partial positive solutions for the conjecture; see [1], [2], [4] and [5]. Furthermore, on the basis of the facts that $x - \ln x$ is increasing for $x > 1$ and $\lambda_1 \geq \bar{d}$, they introduced a new conjecture in [3], which is a generalization of Conjecture 1.1.

Conjecture 1.2. *Let G be a non-singular graph. Then $\mathcal{E}(G) \geq n - 1 + \bar{d}$ except for P_4 and the graph on 4 vertices obtained by adding a pendant edge on a vertex of a triangle.*

Notice that $n - 1 \geq \Delta(G)$ and $\bar{d} \geq \delta(G)$, Conjecture 1.2 is a strengthened version of Conjecture 1.1.

For the Erdös-Rényi-type random graphs, this Conjecture is true. In fact, recall that $\mathcal{G}_{n,p}$ consists of all graphs on n vertices in which the edges are chosen independently with probability p, where $p \in (0, 1)$ is a constant.

Lemma 1.3. *(see [9]) Let $\varepsilon > 0$ be fixed, $\varepsilon n^{-3/2} \leq p \leq 1 - \varepsilon n^{-3/2}$. Let $q = q(n)$ be a natural number and set*

$$\mu_q = nB(q; n - 1, p) \quad \textit{and} \quad \nu_q = n\{1 - B(q + 1; n - 1, p)\},$$

where

$$B(l;m,p)=\sum_{j\geq l} b(j;m,p)$$

in which $b(j;m,p)=\binom{m}{j}p^j(1-p)^{m-j}$ *is subject to the binomial distribution. For a random graph* $G\in\mathcal{G}_{n,p}$, *denote by* $Y_q(G)$ *the number of vertices of degrees at least* q *and* $Z_q(G)$ *the number of vertices of degrees at most* q. *Then*

$$(i)\ \ if\ \ \mu_q\to 0,\ P(Y_q=0)\to 0;\ (ii)\ \ if\ \ \nu_q\to 0,\ P(Z_q=0)\to 0.$$

It is not difficult to check that the minimum and maximum degrees δ and Δ of a random graph G_p on n vertices satisfy that

$$np-n^{\frac{3}{4}}<\delta(G_p)\leq\Delta(G_p)<np+n^{\frac{3}{4}},\ \text{a.s.}$$

(i) and (ii) hold by Chernoff's Inequality.

On the other hand, the asymptotic value of the energy of G_p was calculated in [11] by Du, Li, and Li, see the following.

Theorem 1.4.

$$\mathscr{E}(G_p)=(\frac{8}{3\pi}\sqrt{p(1-p)}+o(1))\cdot n^{3/2}\quad a.s.$$

So, Conjecture 1.2 holds a.s. as $n\to\infty$.

In [3], Akbari et al. did some preliminary study and they managed to show that Conjecture 1.2 holds for regular graphs, bipartite graphs, planar graphs, graphs with $\lambda_1\leq 7.11$, and graphs with $m\leq 2.574n$. In this paper, we consider threshold graphs, which are not contained in any of the graph families above, and we find that except the counterexample mentioned in the conjecture, all threshold graphs satisfy the inequality. So it is impossible to find a similar counterexample in the family of threshold graphs.

Theorem 1.5. *Conjecture 1.2 holds for all non-singular threshold graphs* G *with* $n\geq 5$, *and the inequality holds if and only if* $G\cong K_n$.

The proof will be given in Section 3.

2 Preliminaries

Before giving proof of our main result Theorem 1.5, we need to do some preparations.

Recall that a vertex is isolated in a graph G if it has no neighbors in G, and is dominating if it is adjacent to all other vertices of G. A *threshold graph* is a graph that can be constructed from a graph on one vertex by repeated adding a single isolated vertex or a dominating vertex. Threshold graphs were first introduced by Henderson and Zalcstein in 1977 [14], which later act as a very important role in the domain of algebraic graph theory and computer science. A threshold graph has several equivalent definitions, for example, a graph is a threshold graph if and only if it contains no P_4, C_4 or $P_2 \cup P_2$ as induced subgraph. For more knowledge about threshold graphs, we refer the reader to [12] and [15].

From our definition, we can use a $\{0,\ 1\}$-sequence $b = \{b_1, \dots, b_n\}$ to represent a threshold graph G with $V(G) = \{v_1, \dots, v_n\}$, where $b_1 = 0$, $b_i = 0$ if and only if v_i was added as an isolated vertex, and $b_i = 1$ if and only if v_i was added as a dominating vertex, for $i = 2, \dots, n$. For example, the counterexample mentioned in Conjecture 1.2 is just the threshold graph $\{0, 1, 0, 1\}$.

It is necessary to do some preliminary observation on the objects we are going to deal with. First, we only need to deal with connected threshold graphs, since any disconnected threshold graph contains isolated vertices and is therefore singular. A threshold graph is connected if and only if its $\{0, 1\}$-sequence is ended with 1. Second, if there exist two consecutive 0's in the sequence, their corresponding row vectors in $A(G)$ are identical, making G singular, too. Thus, the sequence can be rewritten as $b = \{0, 1^{s_1}, \dots, 0, 1^{s_k}\}$. In fact, it was calculated in [8] that the determinant of the adjacency matrix of threshold graph G of this form is $\det(A(G) = (-1)^{\sum_{i=1}^{k} s_i} \prod s_i$. So this is just the sufficient and necessary condition of G being non-singular.

Lou et al. in [17] studied the spectral property of threshold graphs, and gave some description of the distribution of eigenvalues of threshold graphs; see the following.

Theorem 2.1. *Let G be a threshold graph with representation sequence $b = \{0, 1^{s_1}, \dots, 0, 1^{s_k}\}$. Then the spectrum of G is*

$$\lambda_1, \dots, \lambda_k, [-1]^{n-2k+1}, \lambda_{n-k+2}, \dots, \lambda_n,$$

where

$$\lambda_1 > \cdots > \lambda_k > \frac{\sqrt{2}-1}{2} > \frac{-\sqrt{2}-1}{2} > \lambda_{n-k+2} > \cdots > \lambda_n.$$

Suppose that A is a symmetric real matrix whose rows and columns are indexed by $X = \{1, \dots, n\}$. Let $\{X_1, \dots, X_m\}$ be a partition of X, and rewrite A according to $\{X_1, \ldots, X_m\}$ as follows:

$$A = \begin{bmatrix} A_{1,1} & \ldots & A_{1,m} \\ \vdots & & \vdots \\ A_{m,1} & \ldots & A_{m,m} \end{bmatrix}$$

where $A_{i,j}$ denotes the block of A formed by rows in X_i and columns in X_j. Let $b_{i,j}$ denote the average row sum of $A_{i,j}$. Then the matrix $B = [b_{i,j}]$ is called the *quotient matrix*. If the row sum of each block $A_{i,j}$ is constant, then the partition is called an *equitable partition*.

Take the partition π in G: $V(G) = \{u_1, \ldots, u_k, V_1, \ldots, V_k\}$, where u_i denotes the k vertices corresponding to 0 and V_i denotes the s_i vertices corresponding to the all 1 segment of length s_i. Then π is an equitable partition of $V(G)$ and the quotient matrix has the form

$$B = \begin{bmatrix} 0 & s_1 & 0 & s_2 & 0 & \cdots & 0 & s_k \\ 1 & s_1 - 1 & 0 & s_2 & 0 & \cdots & 0 & s_k \\ 0 & 0 & 0 & s_2 & 0 & \cdots & 0 & s_k \\ 1 & s_1 & 1 & s_2 - 1 & 0 & \cdots & 0 & s_k \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & s_k \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & s_k \\ 1 & s_1 & 1 & s_2 & 1 & \cdots & 1 & s_k - 1 \end{bmatrix}$$

Theorem 2.2. *Let G be the threshold graph with form $b = \{0, 1^{s_1}, \ldots, 0, 1^{s_k}\}$. The spectrum of B is*

$$\phi_1 > \cdots > \phi_k > \phi_{k+1} = -1 > \phi_{k+2} > \cdots > \phi_{2k},$$

where

$$\phi_j = \lambda_j \quad \text{and} \quad \phi_{k+j} = \lambda_{n-k+j} \quad for \quad j = 1, \ldots, k$$

In the sequel, we also need some lemmas in linear algebra, and the reader can find them in [10].

Lemma 2.3. *(Rayleigh's quotient) Let A be a real $n \times n$ symmetric matrix. The spectral radius of A satisfies that*

$$\rho(A) \geq X^\intercal A X$$

for all unit vectors X, and the equality holds if and only if X is an eigenvector of $\rho(A)$.

Lemma 2.4. *(Interlacing theorem) Let A be a real $n \times n$ symmetric matrix and let B be a principal submatrix of A with order $m \times m$. Then, for $i = 1, \ldots, m$, the eigenvalues of A and B satisfy that*

$$\lambda_{n-m+i}(A) \leq \lambda_i(B) \leq \lambda_i(A).$$

3 Proof of Theorem 1.5

Now we are ready to give the proof of our main result Theorem 1.5.

The degree sequence of $\{0, 1^{s_1}, \ldots, 0, 1^{s_k}\}$ is
$\underbrace{n-1, \ldots, n-1}_{s_k}, \underbrace{n-2, \ldots, n-2}_{s_{k-1}}, \ldots, \underbrace{n-k, \ldots, n-k}_{s_1},$
$n-k = \sum_{i=1}^{k} s_i,\ \sum_{i=2}^{k} s_i,\ \ldots,\ s_{k-1}+s_k,\ s_k,$ and
$\bar{d} = \frac{(n-1-k)(n-k)}{n} + \frac{2}{n}\sum_{i=1}^{k} is_i.$
The inequality we are going to prove is

$$\mathcal{E}(G) \geq n-1+\frac{(n-1-k)(n-k)}{n}+\frac{2}{n}\sum_{i=1}^{k} is_i.$$

Denote $\boldsymbol{j} = \frac{1}{\sqrt{n}}\mathbf{1}$. Notice that $n-1 = \boldsymbol{j}^{\intercal}(J-I)\boldsymbol{j}$, and according to Lemma 2.3, $\lambda_1 > \boldsymbol{j}^{\intercal}A(G)\boldsymbol{j}$ if $G \ncong K_n$. So

$$n-1-\lambda_1 < \frac{2}{n}[\sum_{i=1}^{k}(k-i)s_i + \frac{k(k-1)}{2}] = \frac{2}{n}[k(n-k) - \sum_{i=1}^{k} is_i + \frac{k(k-1)}{2}].$$

Denoting $S = \sum_{i=2}^{k}(|\lambda_i| + |\lambda_{n-k+i}|)$, we now find a sufficient condition of the conjecture, i.e.,

$$S + (n-2k+1) - \frac{(n-1-k)(n-k)}{n} - \frac{2}{n}\sum_{i=1}^{k} is_i \geq \frac{2}{n}[k(n-k) - \sum_{i=1}^{k} is_i + \frac{k(k-1)}{2}],$$

that is,

$$S - 2k + 2 \geq 0.$$

We first deal with the special case that $s_i = 1$ for $i = 1, \ldots, k$. The threshold graph whose sequence is $\{0, 1, 0, 1, \ldots, 0, 1\}$ is called *anti-regular graph.* In this case, $n = 2k$ and we rewrite the anti-regular graph of order $2k$ as Λ_k. It is difficult to calculate the exact eigenvalues of an anti-regular graph, but in [7], Arguila et al. gave a characterization of the spectrum of anti-regular graphs using the Chebyshev polynomial of the second kind.

Theorem 3.1. *$\lambda \neq -1$ is an eigenvalue of Λ_k if and only if*

$$\lambda = \frac{\sin k\theta}{\sin k\theta + \sin(k-1)\theta},$$

where $\theta = \arccos(\frac{1-2\lambda-2\lambda^2}{2\lambda(\lambda+1)})$.

In this theorem, regarding θ as the variable rather than λ, one gets that

$$\lambda = \frac{-(\cos\theta+1) \pm \sqrt{(\cos\theta+1)(\cos\theta+3)}}{2(\cos\theta+1)},$$

and the equation is split into two parts:

$$g_+(\theta) = \frac{-(\cos\theta+1) + \sqrt{(\cos\theta+1)(\cos\theta+3)}}{2(\cos\theta+1)} = \frac{\sin k\theta}{\sin k\theta + \sin(k-1)\theta}$$

and

$$g_-(\theta) = \frac{-(\cos\theta+1) - \sqrt{(\cos\theta+1)(\cos\theta+3)}}{2(\cos\theta+1)} = \frac{\sin k\theta}{\sin k\theta + \sin(k-1)\theta}.$$

Define a function $f(\theta) = \frac{\sin k\theta}{\sin k\theta + \sin(k-1)\theta}$ on $(0, \pi)$. Notice that $\sin k\theta + \sin(k-1)\theta = 2\sin\frac{2k-1}{2}\theta\cos\frac{\theta}{2}$. So, $\{\frac{2j\pi}{2k-1}\}_{j=1}^{k-1}$ are the poles of $f(\theta)$. In each od the segments $(\frac{2j\pi}{2k-1}, \frac{2(j+1)\pi}{2k-1})$ $(j = 0, \ldots, k-2)$ and $(\frac{2(k-1)\pi}{2k-1}, \pi)$,

$$\begin{aligned}
f'(\theta) &= \frac{k\cos k\theta(\sin k\theta + \sin(k-1)\theta) - \sin k\theta(k\cos k\theta + (k-1)\cos(k-1)\theta)}{[\sin k\theta + \sin(k-1)\theta]^2} \\
&= \frac{-k\sin\theta + \sin k\theta\cos(k-1)\theta}{[\sin k\theta + \sin(k-1)\theta]^2} \\
&= \frac{\sin\theta}{[\sin k\theta + \sin(k-1)\theta]^2}[\frac{1}{2}D_{k-1}(\theta) - (k - \frac{1}{2})],
\end{aligned}$$

where $D_{k-1}(\theta)=\dfrac{\sin(2k-1)\theta}{\sin\theta}$ is the Dirichlet kernel of order $k-1$. Remember that $D_{k-1}=1+2\sum_{l=1}^{k-1}\cos 2l\theta<2k-1$. So, $f(\theta)$ is strictly decreasing in each segment, and thus $f^-(\frac{2j\pi}{2k-1})=-\infty$ and $f^+(\frac{2j\pi}{2k-1})=+\infty$. Also, it is not difficult to obtain that $\lim_{\theta\to 0}f(\theta)=\dfrac{k}{2k-1}$ and $\lim_{\theta\to\pi}f(\theta)=k$. Thus, the two values can naturally be regarded as $f(0)$ and $f(\pi)$ without breaking continuity.

It is trivial to check that $g_+(\theta)$ is strictly increasing and $g_-(\theta)$ is strictly decreasing. Moreover,

$$g_+(0)=\frac{\sqrt{2}-1}{2}<f(0),\quad g_+(\pi)=+\infty; g_(0)=\frac{-\sqrt{2}-1}{2}<f(0),\quad g_-(\pi)=-\infty.$$

Combined with the analysis above about $f(\theta)$, it is easy to see that both $g_+(\theta)$ and $g_-(\theta)$ intersect with $f(\theta)$ at exactly one point in every segment $(\frac{2j\pi}{2k-1},\frac{2(j+1)\pi}{2k-1})$ $(j=0,\dots,k-2)$ and $g_+(\theta)$ has an intersection point with $f(\theta)$ in $(\frac{2(k-1)\pi}{2k-1},\pi)$, which indicates the spectral radius ϕ_1 of Λ_k and we do not need to care about it.

Now we can elaborate a lower bound of S for Λ_k as follows:

$$S>\sum_{j=0}^{k-2}|g_-(\frac{2j\pi}{2k-1})|+|g_+(\frac{2j\pi}{2k-1})|=\sum_{j=0}^{k-2}\sqrt{\frac{3+\cos\frac{2j\pi}{2k-1}}{1+\cos\frac{2j\pi}{2k-1}}}$$

$$=\sum_{j=0}^{k-2}\sqrt{1+\frac{2}{1+\cos\frac{2j\pi}{2k-1}}}>\sum_{j=0}^{k-2}\sqrt{1+\frac{1}{(\frac{\pi}{2}\cdot\frac{2j+3}{2k-1})^2}},$$

The last sum can be seen as an upper Darboux sum:

$$\frac{1}{k-\frac{1}{2}}\sum_{j=0}^{k-2}\sqrt{1+\frac{1}{(\frac{\pi}{2}\cdot\frac{2j+3}{2k-1})^2}}>\int_{\frac{3}{2k-1}}^{\frac{2k-2}{2k-1}}\sqrt{1+\frac{1}{(\frac{\pi x}{2})^2}}.$$

The integral $\int_0^1\sqrt{1+\frac{1}{(\frac{\pi x}{2})^2}}$ is divergent at point 0, and so

$$\lim_{k\to\infty}\int_{\frac{3}{2k-1}}^{\frac{2k-2}{2k-1}}\sqrt{1+\frac{1}{(\frac{\pi x}{2})^2}}=+\infty.$$

It can be checked that when $k \geq 23$,

$$\int_{\frac{3}{2k-1}}^{\frac{2k-2}{2k-1}} \sqrt{1+\frac{1}{(\frac{\pi x}{2})^2}} > 2$$

with the aid of MATLAB. As for $k \leq 22$, we have calculated $S-2k+2$ directly and made the following list:

k	$S-2k+2$	k	$S-2k+2$
2	-0.2077	13	7.5720
3	-0.1145	14	8.7176
4	0.1829	15	9.9086
5	0.6357	16	11.1419
6	1.2138	17	12.4150
7	1.8969	18	13.7254
8	2.6702	19	15.0712
9	3.5226	20	16.4504
10	4.4453	21	17.8615
11	5.4315	22	19.3028
12	6.4753		

From which it could be seen that if $k \geq 4$, $S-2k+2>0$, and thus Conjecture 1.2 holds strictly for Λ_k.

For general G with $k \geq 4$, notice that Λ_k is an induced subgraph of G, and thus $A(\Lambda_k)$ is a principal submatrix of $A(G)$. According to Lemma 2.4, for $i = 2, \ldots, k$,

$$\lambda_i(G) \geq \phi_i(\Lambda_k) \quad \textit{and} \quad \phi_{k+i}(\Lambda_k) \geq \lambda_{n-k+i}.$$

Then,

$$\sum_{i=2}^{k}(|\lambda_i(G)|+|\lambda_{n-k+i}(G)|)-2k+2 > \sum_{i=2}^{k}|(\phi_i(\Lambda_k)|+|\phi_{k+i}(\Lambda_k)|)-2k+2>0,$$

and Conjecture 1.2 also holds strictly for G.

Next we deal with the special cases that $k=2$ and $k=3$.

Case 1: $k=2$.

The quotient matrix of G is

$$B_2 = \begin{bmatrix} 0 & s_1 & 0 & s_2 \\ 1 & s_1-1 & 0 & s_2 \\ 0 & 0 & 0 & s_2 \\ 1 & s_1 & 1 & s_2-1 \end{bmatrix},$$

and the inequality of Conjecture 1.2 becomes

$$\mathcal{E}(G) = \mathcal{E}(B_2) + (n-4) \geq (n-1) + \frac{(n-2)(n-3)}{n} + \frac{2}{n}(s_1 + 2s_2).$$

While $\mathcal{E}(B_2) = tr(B_2) + 2 + 2|\lambda_n| = n - 2 + 2|\lambda_n|$, the inequality is equivalent to

$$|\lambda_n| \geq 1 + \frac{1+s_2}{n}.$$

Denote the characteristic polynomial of B_2 by $P_2(\lambda)$. By calculating, $\frac{P_2(\lambda)}{\lambda+1} = \lambda(\lambda+1)(\lambda-n+2) - s_2(\lambda - s_1)$. Writing $x = -1 - \frac{1+s_2}{n}$, we just need to verify that $\frac{P_2(x)}{x+1} \geq 0$.

Taking $s_1 = n - 2 - s_2$ into the expression of $\frac{P_2(x)}{x+1}$, we get

$$h(s_2) = -\frac{1+s_2}{n}(1+\frac{1+s_2}{n})(n-1+\frac{1+s_2}{n}) + s_2(n-1-s_2+\frac{1+s_2}{n}).$$

Differentiating it

$$h'(s_2) = -\frac{3}{n^3}s_2^2 - 2(\frac{3}{n^3}+1)s_2 + (n - \frac{3}{n^3} - 2),$$

we see that $h'(s_2)$ is strictly decreasing in s_2. Since $h'(1) = n - \frac{12}{n^3} - 4 > 0$, and $h'(n-3) = -\frac{3}{n} + \frac{12}{n^2} - \frac{12}{n^3} + 4 - n < 0$, we have that $h(s_2)$ is strictly increasing and then strictly decreasing on $(1, n-3)$. Since $h(1) = n - \frac{8}{n^3} - 4 > 0$, and $h(n-3) = n - 5 + \frac{6}{n} - \frac{12}{n^2} + \frac{8}{n^3} > 0$, we have $\frac{P_2(x)}{x+1} > 0$, and Conjecture 1.2 holds strictly for threshold graphs with $n \geq 5$ and $k = 2$.

Case 2: $k = 3$**.**

The quotient matrix of G is

$$B_3 = \begin{bmatrix} 0 & s_1 & 0 & s_2 & 0 & s_3 \\ 1 & s_1-1 & 0 & s_2 & 0 & s_3 \\ 0 & 0 & 0 & s_2 & 0 & s_3 \\ 1 & s_1 & 1 & s_2-1 & 0 & s_3 \\ 0 & 0 & 0 & 0 & 0 & s_3 \\ 1 & s_1 & 1 & s_2 & 1 & s_3-1 \end{bmatrix}$$

and the inequality of Conjecture 1.2 becomes

$$\mathcal{E}(G) = \mathcal{E}(B_3) + (n-6) \geq (n-1) + \frac{(n-3)(n-4)}{n} + \frac{2}{n}(n-3+s_2+2s_3).$$

While $\mathcal{E}(B_3) = tr(B_3) + 2 + 2(|\lambda_{n-1}| + |\lambda_n|)$, the inequality is equivalent to

$$|\lambda_{n-1}| + |\lambda_n| \geq 2 + \frac{3}{n} + \frac{1}{n}(s_2 + 2s_3). \tag{*}$$

Denote the characteristic polynomial of B_3 by $P_3(\lambda)$. By calculating,

$$\frac{P_3(\lambda)}{\lambda+1} = \lambda(\lambda+1)[\lambda(\lambda+1)(\lambda-n+3)-(s_2+s_3)(\lambda-s_1)]-s_3[\lambda(\lambda+1)(\lambda-s_1-s_2)-s_2(\lambda-s_1)].$$

Since the roots of a general polynomial of degree ≥ 5 cannot be expressed by a formula, it is not wise to deal with $\frac{P_3(\lambda)}{\lambda+1}$ directly, as we have done in **Case 1**. Let us make some observations. Notice that the expression $2 + \frac{3}{n} + \frac{1}{n}(s_2 + 2s_3)$ does not contain s_1, and it is decreasing in n. For any fixed pair (s_2, s_3), we just need to solve the subcase $s_1 = 1$, since if this subcase satisfies $(*)$, then all threshold graphs $\{0, 1^{s_1}, 0, 1^{s_2}, 0, 1^{s_3}\}$ satisfy $(**)$, according to Lemma 1.2, the interlacing theorem. Now take $s_1 = 1$, and the inequality $(*)$ becomes

$$|\lambda_{n-1}| + |\lambda_n| \geq 3 + \frac{s_3-1}{n}. \tag{**}$$

For the same reason, we just need to solve the subcase $s_2 = 1$, and the inequality $(**)$ becomes

$$|\lambda_{n-1}| + |\lambda_n| \geq 4 - \frac{6}{n},$$

and

$$\frac{P_3(\lambda)}{\lambda+1} = \lambda(\lambda+1)[\lambda(\lambda+1)(\lambda-n+3)-(n-4)(\lambda-1)]-(n-5)[\lambda(\lambda+1)(\lambda-2)-(\lambda-1)].$$

Taking $y = -2.8$, we have used MATLAB to obtain that when $n \geq 13$, $\frac{P_3(y)}{y+1} > 0$, implying that $\lambda_n < -2.8$. By Theorem 2.1, $|\lambda_{n-1}| + |\lambda_n| > 2.8 + \frac{1+\sqrt{2}}{2} > 4$.

As for $6 \leq n \leq 12$, we have calculated the energies of $\{0, 1, 0, 1, 0, 1^{s_3}\}$ directly and verified the validity of Conjecture 1.2. Now we make a table of the results as follows:

n	$\mathcal{E}$	$n-1+\bar{d}$
6	8.2892	8
7	10.9185	10.2857
8	13.3330	12.5
9	15.6367	14.6667
10	17.8722	16.8
11	20.0620	18.9091
12	22.2189	21

The proof of Theorem 1.5 is finally complete. ∎

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