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GRAPH ENERGY CHANGE DUE TO ANY SINGLE EDGE DELETION*

WEN-HUAN WANG† AND WASIN SO‡

Abstract. The energy of a graph is the sum of the absolute values of its eigenvalues. We propose a new problem on graph energy change due to any single edge deletion. Then we survey the literature for existing partial solution of the problem, and mention a conjecture based on numerical evidence. Moreover, we prove in three different ways that the energy of a cycle graph decreases when an arbitrary edge is deleted except for the order of 4.

Key words. graph energy change, cycle, path

AMS subject classifications. graph energy change, cycle, path

This paper is dedicated to Professor Ravindra B. Bapat on the occasion of his 60th birthday

1. Introduction. Throughout this paper, G denotes a labeled simple graph on the vertex set $\{1, 2, \dots, n\}$. The adjacency matrix of G is $A(G) = [a_{ij}]$ where $a_{ij} = a_{ji} = 1$ if i and j are adjacent, and $a_{ij} = a_{ji} = 0$ otherwise. The characteristic polynomial of G is $\chi(G) = \det(xI - A(G))$, and the spectrum $Sp(G)$ of G is the collection of all eigenvalues of $A(G)$, which are all real numbers because $A(G)$ is a real symmetric matrix. Graph energy is a concept transplanted from chemistry to mathematics, and its study brings together many areas of mathematics including graph theory, linear algebra, combinatorics, complex analysis, etc. See the book of Gutman, Li, and Shi [13] for the history and development of graph energy up until the year 2012. There are several equivalent definitions of graph energy, the original one is given by Gutman [7] using the spectrum of G.

Definition 1.1. *The energy of G is defined as*

$$\mathcal{E}(G) = |\lambda_1| + \cdots + |\lambda_n|,$$

where $Sp(G) = \{\lambda_1, \dots, \lambda_n\}$.

One area in the study of graph energy, called graph energy change [4, 5, 17], is

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†Department of Mathematics, Shanghai University, Shanghai 200444, China. email: whwang@shu.edu.cn

‡Department of Mathematics, San Jose State University, San Jose, California 95192-0103. email: wasin.so@sjsu.edu

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to understand how graph energy changes when a subgraph is deleted. It becomes especially interesting when the subgraph is just an edge. In his 2001 survey paper [8] on graph energy, Gutman mentioned a "hard-to-crack" problem:

Characterize graphs G and their edges e such that $\mathcal{E}(G-e) \leq \mathcal{E}(G)$.

After 15 years, this problem is still far from fully resolved. Even though some progress was made in the past, the complete characterization seems beyond the currently available techniques. Instead, we study the modified problem:

What are the graphs G with one of the following mutually exclusive properties:

- *energy decreased: $\mathcal{E}(G) > \mathcal{E}(G-e)$ for each edge e,*
- *energy increased: $\mathcal{E}(G) < \mathcal{E}(G-e)$ for each edge e,*
- *energy unchanged: $\mathcal{E}(G) = \mathcal{E}(G-e)$ for each edge e?*

The first family of graphs with the property of energy decreased is the family of forests.

Theorem 1.2. *If G is a forest with at least one edge, then $\mathcal{E}(G) > \mathcal{E}(G-e)$ for each edge e.*

This result was proved by Gutman [6] in 1977 using the Coulson integral formula for trees, see [5] for another proof using singular value inequalities. In 1999, Gutman and Pavlovic [11] computed the explicit formula for the energy of a complete graph with a deleted edge, and found another family of graphs with the property that energy decreases.

Theorem 1.3. *If K_n is the complete graph of order $n \geq 2$, then $\mathcal{E}(K_n) > \mathcal{E}(K_n - e)$ for each edge e.*

Recently, Gutman and Shao [12, Theorem 3.1] proved that oddly even cycles also have the property of energy decreases, using the Coulson integral formula for bipartite graphs.

Theorem 1.4. *If C_{4k+2} is the cycle graph of order $4k+2$ with $k \geq 1$, then $\mathcal{E}(C_{4k+2}) > \mathcal{E}(C_{4k+2} - e)$ for each edge e.*

A main goal of this paper is to generalize this result to any cycle C_n except $n = 4$.

Theorem 1.5. *Let C_n be the cycle graph of order $n \geq 3$. If $n \neq 4$, then $\mathcal{E}(C_n) > \mathcal{E}(C_n - e)$ for each edge e.*

Note that $C_n - e = P_n$, where P_n is the path graph of order n. Hence, Theorem 1.5 states that cycles have more energy than paths except order 4. Indeed Theorem 1.5 was already anticipated by Gutman, Milun and Trinajstic [9] from a chemical perspective. They actually provided numerical evidence, but no formal proof was

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recorded. We provide three proofs of Theorem 1.5 using different approaches. In Section 2, we give the first proof based on trigonometric inequalities after getting explicit formulas for the energy of path and cycle. The second proof based on matching numbers of path and cycle is presented in Section 3. In Section 4, we present the last proof using the recursion formula for the characteristic polynomial of a path.

The following observation of Cioăba [5] provides an infinite family of graphs with the property of increasing energy, and also shed some light on the exceptional case $n = 4$ in Theorem 1.5 (note that $C_4 = K_{2,2}$).

THEOREM 1.6. *If $K_{n,n}$ is the regular complete bipartite graph of order $2n$ with $n \geq 2$, then $\mathcal{E}(K_{n,n}) < \mathcal{E}(K_{n,n} - e)$ for each edge e.*

The proof [5, Example 4.6] of Theorem 1.6 first explicitly computes the spectra of $K_{n,n}$ and $K_{n,n} - e$, and then obtains closed forms of $\mathcal{E}(K_{n,n})$ and $\mathcal{E}(K_{n,n} - e)$ for comparison. This result is a special case of the following theorem of Akbari, Ghorbani and Oboudi [2], whose proof avoids the difficult calculation of eigenvalues.

THEOREM 1.7. *If $K_{t_1,\ldots,t_k}$ is the complete multipartite graph with $k \geq 2, t_i \geq 2$, then $\mathcal{E}(K_{t_1,\ldots,t_k}) < \mathcal{E}(K_{t_1,\ldots,t_k} - e)$ for any edge e.*

There are infinite graphs G [15] with a special (not arbitrary) edge e such that $\mathcal{E}(G - e) = \mathcal{E}(G)$, but it seems that there is NO graph G with the property that $\mathcal{E}(G - e) = \mathcal{E}(G)$ for **each** edge e. Therefore we suggest the following.

CONJECTURE 1.8. *There is no graph G such that $\mathcal{E}(G - e) = \mathcal{E}(G)$ for each edge e.*

Of course, it suffices to check connected graphs for counterexamples if they exist. The authors searched by computer through all connected graphs of order up to 11, which amounts to more than one billion graphs. No counterexample was found. Moreover, since the deletion of a cut-edge from a graph decreases its energy [5, Theorem 4.2], a counterexample to Conjecture 1.8 cannot have any cut-edge.

2. Proof by trigonometry. Recall from [3] that

$$Sp(P_n) = \{2\cos\frac{j\pi}{n+1} : j = 1, 2, \ldots, n\},$$

and

$$Sp(C_n) = \{2\cos\frac{2j\pi}{n} : j = 1, 2, \ldots, n\}.$$

Then, by Definition 1.1 and trigonometric summation formulas, we have [7, page 14]

$$\mathcal{E}(P_n) = \begin{cases} 2\cot\frac{\pi}{2n+2} - 2 & \text{if } n \equiv 1 \ (mod\ 2) \\ 2\csc\frac{\pi}{2n+2} - 2 & \text{if } n \equiv 0 \ (mod\ 2), \end{cases}$$

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and [1]

$$\mathcal{E}(C_n) = \begin{cases} 2\csc\frac{\pi}{2n} & \text{if } n \equiv 1 \ (mod\ 2) \\ 4\csc\frac{\pi}{n} & \text{if } n \equiv 2 \ (mod\ 4) \\ 4\cot\frac{\pi}{n} & \text{if } n \equiv 0 \ (mod\ 4). \end{cases}$$

We need some inequalities to help prove Theorem 1.5.

Lemma 2.1. *For fixed $k > 0$, $a < b$ if and only if $\frac{a}{k+a} < \frac{b}{k+b}$ provided that both $k+a$ and $k+b$ are nonzero.*

Lemma 2.2.

(i) For $x > 0$, $\sin x < x$.
(ii) For $0 < x < \frac{\pi}{2}, x < \tan x$.

Lemma 2.3. *For $x > 0$, $x - \frac{1}{6}x^3 < \sin x$.*

Proof. Consider the function $f(x) = \sin x - x + \frac{1}{6}x^3$ for $x \geq 0$. For $x > 0$, $f'(x) = \cos x - 1 + \frac{1}{2}x^2 = 2(\frac{x}{2} + \sin\frac{x}{2})(\frac{x}{2} - \sin\frac{x}{2}) > 0$, by Lemma 2.2 (i). Hence, for $x > 0$, $f(x) > f(0) = 0$, i.e., $x - \frac{1}{6}x^3 < \sin x$. ∎

Lemma 2.4. *For $0 < x < \sqrt{2}$, $\tan x < \frac{2x}{2-x^2}$.*

Proof. Consider the function $f(x) = 2x\cos x - (2-x^2)\sin x$ for $0 \leq x < \sqrt{2}$. For $0 < x < \sqrt{2}$, $f'(x) = x^2\cos x > 0$, and hence $f(x) > f(0) = 0$, i.e. $(2-x^2)\sin x < 2x\cos x$. Consequently, $\tan x < \frac{2x}{2-x^2}$. ∎

First proof of Theorem 1.5:

Case 1: $n \equiv 1 \ (mod\ 2)$

It suffices to show that $2\csc\frac{\pi}{2n} > 2\cot\frac{\pi}{2n+2} - 2$ or equivalently, $\tan\frac{\pi}{2n+2} > \frac{\sin\frac{\pi}{2n}}{1+\sin\frac{\pi}{2n}}$ for $n \geq 3$. Now

$$\tan\frac{\pi}{2n+2} > \frac{\pi}{2n+2} > \frac{\pi}{2n+\pi} = \frac{\pi/2n}{1+\pi/2n} > \frac{\sin\frac{\pi}{2n}}{1+\sin\frac{\pi}{2n}},$$

where the first inequality is due to Lemma 2.2 (ii) (with $x = \frac{\pi}{2n+2}$), and the last inequality is due to Lemma 2.2 (i) (with $x = \frac{\pi}{2n}$) and Lemma 2.1 (with $k = 1$, $a = \sin\frac{\pi}{2n}$, and $b = \frac{\pi}{2n}$).

Case 2: $n \equiv 0 \ (mod\ 4)$

It suffices to show that $4\cot\frac{\pi}{n} > 2\csc\frac{\pi}{2n+2} - 2$ for $n \geq 8$. Indeed, it can be verified numerically for $n = 8, 9$. For $n \geq 10$, we have equivalently

$$\sin\frac{\pi}{2n+2} > \frac{\tan\frac{\pi}{n}}{2+\tan\frac{\pi}{n}}.$$

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Now $n \geq 10 > 8 \approx \frac{\pi^2}{8(\pi-2-\pi^2/10)}$, and so we have $\frac{\pi-2-\pi^2/10}{3n} > \frac{\pi^2}{24n^2}$. Hence

$$\frac{\pi-2-\pi^2/n}{2n+\pi-\pi^2/n} \geq \frac{\pi-2-\pi^2/10}{2n+\pi-\pi^2/n} > \frac{\pi-2-\pi^2/10}{3n} > \frac{\pi^2}{24n^2} > \frac{\pi^2}{6(2n+2)^2}$$

and so

$$\frac{\pi}{2n+2} - \frac{1}{6}\left(\frac{\pi}{2n+2}\right)^3 > \frac{\pi}{2n+\pi-\pi^2/n}.$$

Consequently,

$$\sin\frac{\pi}{2n+2} > \frac{\pi}{2n+2} - \frac{1}{6}\left(\frac{\pi}{2n+2}\right)^3 > \frac{\pi}{2n+\pi-\pi^2/n} > \frac{\tan\frac{\pi}{n}}{2+\tan\frac{\pi}{n}},$$

where the first inequality is due to Lemma 2.3 (with $x = \frac{\pi}{2n+2}$), and the last inequality is due to Lemma 2.4 (with $x = \frac{\pi}{n} < \frac{\pi}{10} < \sqrt{2}$) and Lemma 2.1 (with $k = 2$, $a = \tan\frac{\pi}{n}$, and $b = \frac{2\pi/n}{2-(\pi/n)^2}$).

Case 3: $n \equiv 2\ (mod\ 4)$

It suffices to show that $4\csc\frac{\pi}{n} > 2\csc\frac{\pi}{2n+2} - 2$ for $n \geq 6$. Indeed, it can be verified numerically for $n = 6, 7, 8, 9$. For $n \geq 10$, we have equivalently

$$\sin\frac{\pi}{2n+2} > \frac{\sin\frac{\pi}{n}}{2+\sin\frac{\pi}{n}}.$$

To see this, by Case 2, it suffices to show that

$$\frac{\tan\frac{\pi}{n}}{2+\tan\frac{\pi}{n}} > \frac{\sin\frac{\pi}{n}}{2+\sin\frac{\pi}{n}},$$

which follows easily from Lemma 2.2 (i) and (ii) (with $x = \frac{\pi}{n} < \frac{\pi}{2}$) and Lemma 2.1 (with $k = 2$, $a = \tan\frac{\pi}{n}$, and $b = \sin\frac{\pi}{n}$). ◻

3. Proof by combinatorics.

By interpreting eigenvalues as roots of the characteristic polynomial and using complex analysis, there is an equivalent definition for graph energy [10] as follows.

Definition 3.1.

$$\mathcal{E}(G) = \frac{1}{\pi}\int_0^\infty \frac{1}{y^2}\ln[(a_0 - a_2y^2 + a_4y^4 - \cdots)^2 + (a_1y - a_3y^3 + a_5y^5 - \cdots)^2]\,dy,$$

where $\chi(G) = a_0x^n + a_1x^{n-1} + \cdots + a_kx^{n-k} + \cdots + a_n$ *with* $a_0 = 1$.

Example 3.2. *(i) Since* $\chi(P_3) = x^3 - 2x$,

$$\mathcal{E}(P_3) = \frac{1}{\pi}\int_0^\infty \frac{1}{y^2}\ln[(1+2y^2)^2]\,dy = \frac{2\sqrt{2}}{\pi}\int_0^\infty \frac{1}{u^2}\ln[1+u^2]\,du = 2\sqrt{2}.$$

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(ii) Since $\chi(C_4) = x^4 - 4x^2$,

$$\mathcal{E}(C_4) = \frac{1}{\pi}\int_0^\infty \frac{1}{y^2}\ln[(1+4y^2)^2]\,dy = \frac{4}{\pi}\int_0^\infty \frac{1}{u^2}\ln[1+u^2]\,du = 4.$$

To use this definition, we need to compute the characteristic polynomial of G effectively. By Sachs Theorem [3], for $i \geq 1$,

$$a_i = \sum_{S\in L_i(G)} (-1)^{\omega(S)} 2^{c(S)},$$

where $L_i(G)$ is the collection of linear subgraphs S (of order i) in G, $\omega(S)$ is the number of components in S, $c(S)$ is the number of cycles in S.

Let $m(G,k)$ be the number of k-matchings in G with the convention that for $k < 0$, $m(G,0) = 1$ and $m(G,k) = 0$. According to Riordan [16], the following explicit formulas are due to I. Kaplansky.

$$m(P_n,k) = \binom{n-k}{k} \quad \text{for } 2k \leq n,$$

and

$$m(C_n,k) = \binom{n-k}{k} + \binom{n-k-1}{k-1} \quad \text{for } 2k \leq n.$$

Clearly, we have $m(C_n,k) \geq m(P_n,k)$.

Lemma 3.3. $\mathcal{E}(P_n) = \frac{1}{\pi}\int_0^\infty \frac{1}{y^2}\ln[(m(P_n,0) + m(P_n,1)y^2 + \cdots + m(P_n,k)y^{2k} + \cdots)^2]\,dy$.

Proof. For P_n, we have

$$a_i = \sum_{S\in L_i(P_n)} (-1)^{\omega(S)} 2^{c(S)} = \sum_{S=\frac{i}{2}-\text{matching}} (-1)^{\omega(S)}$$
$$= \begin{cases} 0 & \text{if } i = \text{odd} \leq n, \\ (-1)^k m(P_n,k) & \text{if } i = 2k \leq n. \end{cases}$$

Hence, $a_i = 0$ for $i =$ odd, and $a_{2k} = (-1)^k m(P_n,k)$ for $2k \leq n$. Consequently, by Definition 3.1, we have the required result. □

Lemma 3.4. *For integer* $h \geq 1$,

(i) $\mathcal{E}(C_{2h+1}) = \frac{1}{\pi}\int_0^\infty \frac{1}{y^2}\ln[(\sum_{k=0}^{h} m(C_{2h+1},k)y^{2k})^2 + (2y^{2h+1})^2]\,dy$.

(ii) $\mathcal{E}(C_{4h+2}) = \frac{1}{\pi}\int_0^\infty \frac{1}{y^2}\ln[(\sum_{k=0}^{2h} m(C_{4h+2},k)y^{2k} + 4y^{4h+2})^2]\,dy$.

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(iii) $\mathcal{E}(C_{4h}) = \frac{1}{\pi}\int_0^{\infty} \frac{1}{y^2} \ln[(\sum_{k=0}^{2h-1} m(C_{4h},k)y^{2k})^2]\, dy$.

Proof. For C_n, we have

$$\begin{aligned} a_i &= \sum_{S\in L_i(C_n)} (-1)^{\omega(S)} 2^{c(S)} = \sum_{S=\frac{i}{2}-\text{matching}} (-1)^{\omega(S)} \\ &= \begin{cases} 0 & \text{if } i = \text{odd} < n, \\ (-1)^k m(C_n,k) & \text{if } i = 2k < n, \end{cases} \end{aligned}$$

and

$$\begin{aligned} a_n &= \sum_{S\in L_n(C_n)} (-1)^{\omega(S)} 2^{c(S)} \\ &= \sum_{S=\frac{n}{2}-\text{matching}} (-1)^{\omega(S)} + \sum_{S=C_n} (-1)^1 2^1 \\ &= (-1)^{\frac{n}{2}} m(C_n, \frac{n}{2}) - 2 \\ &= \begin{cases} 0 & \text{if } \frac{n}{2} = \text{even}, \\ -4 & \text{if } \frac{n}{2} = \text{odd}, \\ -2 & \text{if } n = \text{odd}. \end{cases} \end{aligned}$$

Consequently, by Definition 3.1, the required results follow. □

Second proof of Theorem 1.5:

Case 1: $n \equiv 1\ (mod\ 2)$, i.e., $n = 2h+1$ for $h \geq 1$.
Since $m(P_{2h+1},k) \leq m(C_{2h+1},k)$ for any k,

$$\left(\sum_{k=0}^{h} m(P_{2h+1},k)y^{2k}\right)^2 < \left(\sum_{k=0}^{h} m(C_{2h+1},k)y^{2k}\right)^2 + \left(2y^{2h+1}\right)^2.$$

Hence we have $\mathcal{E}(P_n) < \mathcal{E}(C_n)$ by Lemmas 3.3 and 3.4 (i).

Case 2: $n \equiv 2\ (mod\ 4)$, i.e., $n = 4h+2$ for $h \geq 1$.
Since $m(P_{4h+2},k) \leq m(C_{4h+2},k)$ for any k,

$$\begin{aligned} \left(\sum_{k=0}^{2h+1} m(P_{4h+2},k)y^{2k}\right)^2 &= \left(\sum_{k=0}^{2h} m(P_{4h+2},k)y^{2k} + y^{4h+2}\right)^2 \\ &< \left(\sum_{k=0}^{2h} m(C_{4h+2},k)y^{2k} + 4y^{4h+2}\right)^2. \end{aligned}$$

Hence we have $\mathcal{E}(P_n) < \mathcal{E}(C_n)$ by Lemmas 3.3 and 3.4 (ii).

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Case 3: $n \equiv 0\ (mod\ 4)$, i.e., $n = 4h$ for $h \geq 2$.
We want to prove, by Lemmas 3.3 and 3.4 (iii),

$$\begin{aligned}\mathcal{E}(P_{4h}) &= \frac{2}{\pi}\int_0^{\infty}\frac{1}{y^2}\ln[\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}]\,dy\\ &< \frac{2}{\pi}\int_0^{\infty}\frac{1}{y^2}\ln[\sum_{k=0}^{2h-1} m(C_{4h},k)y^{2k}]\,dy = \mathcal{E}(C_{4h}).\end{aligned}$$

It suffices to show that, for $h \geq 2$,

$$\mathcal{E}(C_{4h}) - \mathcal{E}(P_{4h}) \leq \mathcal{E}(C_{4h+4}) - \mathcal{E}(P_{4h+4}),$$

because

$$0 < 0.139313 = 9.65685 - 9.51754 \approx \mathcal{E}(C_8) - \mathcal{E}(P_8).$$

To this end, we need

$$\frac{\sum_{k=0}^{2h-1} m(C_{4h},k)y^{2k}}{\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}} \leq \frac{\sum_{k=0}^{2h+1} m(C_{4h+4},k)y^{2k}}{\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}},$$

which is proved in Lemma 3.9 after a series of preliminary lemmas on matching numbers of paths and cycles.

Lemma 3.5. *For integers $a, b, c, d, r \geq 1$ such that $a + b = c + d$, we have*

$$m(P_a \cup P_b, r) - m(P_c \cup P_d, r) = (-1)^x[m(P_{a-x} \cup P_{b-x}, r-x) - m(P_{c-x} \cup P_{d-x}, r-x)]$$

for $1 \leq x \leq r$.

Proof. Applying the recursive formula:

$$m(G,r) = m(G-uv,r) + m(G-u-v,r-1)$$

to both P_{a+b} and P_{c+d}, we obtain

$$\begin{aligned}&m(P_a \cup P_b, r) + m(P_{a-1} \cup P_{b-1}, r-1)\\ &= m(P_{a+b}, r)\\ &= m(P_{c+d}, r)\\ &= m(P_c \cup P_d, r) + m(P_{c-1} \cup P_{d-1}, r-1).\end{aligned}$$

It follows that

$$m(P_a \cup P_b, r) - m(P_c \cup P_d, r) = (-1)[m(P_{a-1} \cup P_{b-1}, r-1) - m(P_{c-1} \cup P_{d-1}, r-1)]$$

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and then, by induction, we have

$m(P_a \cup P_b, r) - m(P_c \cup P_d, r) = (-1)^x [m(P_{a-x} \cup P_{b-x}, r-x) - m(P_{c-x} \cup P_{d-x}, r-x)]$

for $1 \le x \le r$. $\square$

LEMMA 3.6. *For integer $h \ge 1$,*

(i) $m(P_{4h-2} \cup P_{4h+4}, k) = m(P_{4h} \cup P_{4h+2}, k)$ *for* $0 \le k \le 4h-2$.

(ii) $m(P_{4h-2} \cup P_{4h+4}, 4h-1) = m(P_{4h} \cup P_{4h+2}, 4h-1) + 1$.

(iii) $m(P_{4h-2} \cup P_{4h+4}, 4h) = m(P_{4h} \cup P_{4h+2}, 4h) + 2$.

(iv) $m(P_{4h-2} \cup P_{4h+4}, 4h+1) = m(P_{4h} \cup P_{4h+2}, 4h+1)$.

Proof. (i) For $k \le 4h-2$, we have $4h-2-k, 4h+4-k, 4h-k, 4h+2-k \ge 0$. By Lemma 3.5 with $x = k$,

$$\begin{aligned} &m(P_{4h-2} \cup P_{4h+4}, k) - m(P_{4h} \cup P_{4h+2}, k) \\ &= (-1)^k [m(P_{4h-2-k} \cup P_{4h+4-k}, 0) - m(P_{4h-k} \cup P_{4h+2-k}, 0)] \\ &= (-1)^k [1-1] = 0. \end{aligned}$$

(ii) By Lemma 3.5 with $x = 4h-2$,

$$\begin{aligned} &m(P_{4h-2} \cup P_{4h+4}, 4h-1) - m(P_{4h} \cup P_{4h+2}, 4h-1) \\ &= (-1)^{4h-2} [m(P_0 \cup P_6, 1) - m(P_2 \cup P_4, 1)] = 5-4 = 1. \end{aligned}$$

(iii) By Lemma 3.5 with $x = 4h-2$,

$$\begin{aligned} &m(P_{4h-2} \cup P_{4h+4}, 4h) - m(P_{4h} \cup P_{4h+2}, 4h) \\ &= (-1)^{4h-2} [m(P_0 \cup P_6, 2) - m(P_2 \cup P_4, 2)] = 6-4 = 2. \end{aligned}$$

(iv) By Lemma 3.5 with $x = 4h-2$,

$$\begin{aligned} &m(P_{4h-2} \cup P_{4h+4}, 4h+1) - m(P_{4h} \cup P_{4h+2}, 4h+1) \\ &= (-1)^{4h-2} [m(P_0 \cup P_6, 3) - m(P_2 \cup P_4, 3)] = 1-1 = 0. \end{aligned}$$

$\square$

LEMMA 3.7. *For an integer h with $h \ge 2$,*

$$\begin{aligned} &\left[\sum_{k=0}^{2h-1} m(P_{4h-2}, k) y^{2k}\right] \left[\sum_{k=0}^{2h+2} m(P_{4h+4}, k) y^{2k}\right] \\ &= \left[\sum_{k=0}^{2h} m(P_{4h}, k) y^{2k}\right] \left[\sum_{k=0}^{2h+1} m(P_{4h+2}, k) y^{2k}\right] + y^{8h-2} + 2y^{8h}. \end{aligned}$$

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Proof. Note that

$$\begin{aligned}
&\left[\sum_{k=0}^{2h-1} m(P_{4h-2},k)y^{2k}\right]\left[\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}\right]\\
&= \sum_{k=0}^{4h+1} m(P_{4h-2}\cup P_{4h+4},k)y^{2k}\\
&= \sum_{k=0}^{4h+1} m(P_{4h}\cup P_{4h+2},k)y^{2k}+y^{8h-2}+2y^{8h}\\
&= \left[\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}\right]\left[\sum_{k=0}^{2h+1} m(P_{4h+2},k)y^{2k}\right]+y^{8h-2}+2y^{8h},
\end{aligned}$$

where the first and last equalities are due to the identity

$$m(G\cup H,k)=\sum_{i+j=k} m(G,i)m(H,j),$$

and the second equality follows from Lemma 3.6. ∎

Lemma 3.8. *For integer $h\geq 2$,*

$$y^{4h}+2y^{4h+2}+2y^4\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}\leq 2\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}.$$

Proof. For $0\leq k\leq 2h$, we use Kaplansky's formula to obtain

$$m(P_{4h+4},k+2)-m(P_{4h},k)=\frac{2(4h-k)!}{(4h-2k)!\,(k+2)!}(4h+3)(2h-k)\geq 0,$$

hence $m(P_{4h+4},k+2)\geq m(P_{4h},k)$. Moreover,

$$m(P_{4h+4},2h)-m(P_{4h},2h-2)=\frac{(h+1)(2h+1)(4h+3)}{3}\geq 1$$

and

$$m(P_{4h+4},2h+1)-m(P_{4h},2h-1)=4h+3\geq 2.$$

Consequently, the LHS coefficents are always less than or equal to RHS coefficients.
∎

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LEMMA 3.9. *For each integer $h \geq 2$,*

$$\left[\sum_{k=0}^{2h-1} m(C_{4h},k)y^{2k}\right]\left[\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}\right] \leq \left[\sum_{k=0}^{2h+1} m(C_{4h+4},k)y^{2k}\right]\left[\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}\right].$$

Proof. The required inequality is equivalent to

$$\left[\sum_{k=0}^{2h} m(C_{4h},k)y^{2k}\right]\left[\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}\right] + 2y^{4h+4}\left[\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}\right]$$
$$\leq \left[\sum_{k=0}^{2h+2} m(C_{4h+4},k)y^{2k}\right]\left[\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}\right] + 2y^{4h}\left[\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}\right].$$

Apply the formula: $m(C_n,k) = m(P_n,k)+m(P_{n-2},k-1)$ to both sides and cancel the common term $\left[\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}\right]\left[\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}\right]$, the required inequality is now equivalent to

$$\left[\sum_{k=0}^{2h} m(P_{4h-2},k-1)y^{2k}\right]\left[\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}\right] + 2y^{4h+4}\left[\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}\right]$$
$$\leq \left[\sum_{k=0}^{2h+2} m(P_{4h+2},k-1)y^{2k}\right]\left[\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}\right] + 2y^{4h}\left[\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}\right]$$

i.e.,

$$\left[\sum_{k=0}^{2h-1} m(P_{4h-2},k)y^{2k}\right]\left[\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}\right] + 2y^{4h+2}\left[\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}\right]$$
$$\leq \left[\sum_{k=0}^{2h+1} m(P_{4h+2},k)y^{2k}\right]\left[\sum_{k=0}^{2h} m(P_{4h},k)y^{2k}\right] + 2y^{4h-2}\left[\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}\right].$$

By Lemma 3.7, it is equivalent to

$$y^{8h-2} + 2y^{8h} + 2y^{4h+2}\sum_{k=0}^{2h} m(P_{4h},k)y^{2k} \leq 2y^{4h-2}\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k}$$

or

$$y^{4h} + 2y^{4h+2} + 2y^{4}\sum_{k=0}^{2h} m(P_{4h},k)y^{2k} \leq 2\sum_{k=0}^{2h+2} m(P_{4h+4},k)y^{2k},$$

which is true by Lemma 3.8. ☐

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4. Proof by analysis. For comparing energy of two graphs, we have the following Coulson-Jacob formula [8]:

$$\mathcal{E}(G_1) - \mathcal{E}(G_2) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \ln\left|\frac{\chi(G_1, \mathbf{i}x)}{\chi(G_2, \mathbf{i}x)}\right| dx,$$

where G_1 and G_2 are two graphs with the same number of vertices, and $\mathbf{i} = \sqrt{-1}$. Using the recurrsive relation [3] $\chi(P_n, z) = z\chi(P_{n-1}, z) - \chi(P_{n-2}, z)$, Ji and Li [14] proved that

$$\chi(P_n, z) = B_1(z)Y_1^n(z) + B_2(z)Y_2^n(z),$$

where $Y_1(z) = \frac{z+\sqrt{z^2-4}}{2}$, $Y_2(z) = \frac{z-\sqrt{z^2-4}}{2}$, $B_1(z) = \frac{Y_1(z)(z^2-1)-z}{Y_1^3(z)-Y_1(z)}$, and $B_2(z) = \frac{Y_2(z)(z^2-1)-z}{Y_2^3(z)-Y_2(z)}$. Hence

$$\chi(C_n, z) = \chi(P_n, z) - \chi(P_{n-2}, z) - 2 = Y_1^n(z) + Y_2^n(z) - 2.$$

LEMMA 4.1. *For $x \in \mathbb{R}$, define $Z_1(x) = \frac{x+\sqrt{x^2+4}}{2}$, and $Z_2(x) = \frac{x-\sqrt{x^2+4}}{2}$. Then*

(i) *$Z_1(x) + Z_2(x) = x$, $Z_1(x)Z_2(x) = -1$, and $Z_1(-x) = -Z_2(x)$.*
(ii) *For $x > 0$, $Z_1(x) > 1$, and $-1 < Z_2(x) < 0$.*
(iii) *For $x < 0$, $0 < Z_1(x) < 1$, and $Z_2(x) < -1$.*

Proof. Direct verification. □

LEMMA 4.2. *For $x \in \mathbb{R}$, define*

$$C_1(x) = \frac{Z_1(x)(x^2+1)+x}{Z_1^3(x)+Z_1(x)}, \text{ and}$$
$$C_2(x) = \frac{Z_2(x)(x^2+1)+x}{Z_2^3(x)+Z_2(x)}.$$

Then

(i) *$C_1(-x) = C_2(x)$.*
(ii) *$0 < C_1(x), C_2(x) < 1$.*

Proof. (i) It follows from Lemma 4.1 (i) that

$$C_1(-x) = \frac{Z_1(-x)(x^2+1)-x}{Z_1^3(-x)+Z_1(-x)} = \frac{Z_2(x)(x^2+1)+x}{Z_2^3(x)+Z_2(x)} = C_2(x).$$

(ii) Case 1: $x > 0$. Since $Z_1(x) > 1$, we have $C_1(x) > 0$. Moreover, $C_2(x) = \frac{1}{Z_2^2(x)+1}(x^2+1+\frac{x}{Z_2(x)}) > 0$ because $x^2+1 > \frac{x(x+\sqrt{x^2+4})}{2} = xZ_1(x) = -\frac{x}{Z_2(x)}$. Note that $x < \frac{1}{2}(3x+\sqrt{4+x^2}) = Z_1^3(x) - Z_1(x)x^2$, and so $Z_1(x)(x^2+1)+x < Z_1^3(x)+Z_1(x)$.

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Hence $C_1(x) = \frac{Z_1(x)(x^2+1)+x}{Z_1^3(x)+Z_1(x)} < 1$ because $Z_1(x) > 1$ is positive. Also note that $x > \frac{1}{2}(3x - \sqrt{4+x^2}) = Z_2^3(x) - Z_2(x)x^2$, and so $Z_2(x)(x^2+1) + x > Z_2^3(x) + Z_2(x)$. Hence $C_2(x) = \frac{Z_2(x)(x^2+1)+x}{Z_2^3(x)+Z_2(x)} < 1$ because $-1 < Z_2(x) < 0$ is negative. Consequently, we have $0 < C_1(x), C_2(x) < 1$.

Case 2: $x < 0$. It follows from (i) and Case 1 that we also have $0 < C_1(x), C_2(x) < 1$ for $x < 0$.

Case 3: $x = 0$. $0 < C_1(0) = C_2(0) = \frac{1}{2} < 1$. □

Lemma 4.3. *For integer $h \geq 1$ and $x \in \mathbb{R}$, we have*

(i) *for $n = 2h+1$,*

$$\chi(P_n, \boldsymbol{i}x) = (-1)^h \boldsymbol{i}[C_1(x)Z_1^n(x) + C_2(x)Z_2^n(x)]$$

and

$$\chi(C_n, \boldsymbol{i}x) = (-1)^h \boldsymbol{i}[Z_1^n(x) + Z_2^n(x)] - 2,$$

(ii) *for $n = 4h+2$,*

$$\chi(P_n, \boldsymbol{i}x) = -C_1(x)Z_1^n(x) - C_2(x)Z_2^n(x)$$

and

$$\chi(C_n, \boldsymbol{i}x) = -Z_1^n(x) - Z_2^n(x) - 2,$$

(iii) *for $n = 4h$,*

$$\chi(P_n, \boldsymbol{i}x) = C_1(x)Z_1^n(x) + C_2(x)Z_2^n(x)$$

and

$$\chi(C_n, \boldsymbol{i}x) = Z_1^n(x) + Z_2^n(x) - 2.$$

Proof. Use the fact that $Y_1(\mathbf{i}x) = Z_1(x)\mathbf{i}$, $Y_2(\mathbf{i}x) = Z_2(x)\mathbf{i}$, $B_1(\mathbf{i}x) = C_1(x)$, and $B_2(\mathbf{i}x) = C_2(x)$. □

Lemma 4.4. *For integer $h \geq 1$ and nonzero $x \in \mathbb{R}$,*

$$\chi(C_{4h+4}, \boldsymbol{i}x)\chi(P_{4h}, \boldsymbol{i}x) > \chi(P_{4h+4}, \boldsymbol{i}x)\chi(C_{4h}, \boldsymbol{i}x).$$

Proof. Define $f_h(x) = \chi(C_{4h+4}, \mathbf{i}x)\chi(P_{4h}, \mathbf{i}x) - \chi(P_{4h+4}, \mathbf{i}x)\chi(C_{4h}, \mathbf{i}x)$. Using Lemma 4.3 (iii), we have $f_h(x) =$

$$[C_2(x)-C_1(x)][Z_1^4(x)-Z_2^4(x)]+2C_1(x)(Z_1^4(x)-1)Z_1^{4h}(x)+2C_2(x)(Z_2^4(x)-1)Z_2^{4h}(x).$$

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Hence

$$f_{h+1}(x) - f_h(x) = 2C_1(x)(Z_1^4(x)-1)^2 Z_1^{4h}(x) + 2C_2(x)(Z_2^4(x)-1)^2 Z_2^{4h}(x) \geq 0$$

due to Lemma 4.2 (ii). Also note that $f_1(x) = 12x^2 + 27x^4 + 14x^6 + 2x^8$. Finally, $f_h(x) \geq f_1(x) > 0$ for $x \neq 0$. ▯

Third proof Theorem 1.5:

Case 1: $n = 2h+1$ with $h \geq 2$

Since

$$\begin{aligned}|(-1)^h \mathbf{i}(Z_1^n(x) + Z_2^n(x)) - 2| &= \sqrt{(Z_1^n(x) + Z_2^n(x))^2 + 4} \\ &= \sqrt{Z_1^{2n}(x) + Z_2^{2n}(x) + 2} \\ &> \sqrt{C_1^2(x)Z_1^{2n}(x) + C_2^2(x)Z_2^{2n}(x) - 2C_1(x)C_2(x)} \\ &= |C_1(x)Z_1^n(x) + C_2(x)Z_2^n(x)|,\end{aligned}$$

we have

$$\mathcal{E}(C_n) - \mathcal{E}(P_n) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \ln\left|\frac{(-1)^h \mathbf{i}(Z_1^n(x) + Z_2^n(x)) - 2}{C_1(x)Z_1^n(x) + C_2(x)Z_2^n(x)}\right| dx > 0.$$

Case 2: $n = 4h+2$ with $h \geq 1$

Since $|Z_1^n(x) + Z_2^n(x) + 2| > |C_1(x)Z_1^n(x) + C_2(x)Z_2^n(x)|$, we have

$$\mathcal{E}(C_n) - \mathcal{E}(P_n) = \frac{1}{\pi}\int_{-\infty}^{+\infty} \ln\left|\frac{Z_1^n(x) + Z_2^n(x) + 2}{C_1(x)Z_1^n(x) + C_2(x)Z_2^n(x)}\right| dx > 0.$$

Case 3: $n = 4h$ with $h \geq 2$

By Lemma 4.4, for $x \neq 0$,

$$\chi(C_{4h+4}, \mathbf{i}x)\chi(P_{4h}, \mathbf{i}x) > \chi(P_{4h+4}, \mathbf{i}x)\chi(C_{4h}, \mathbf{i}x)$$

and so, by the Coulson-Jacob formula,

$$\mathcal{E}(C_{4h+4}) - \mathcal{E}(P_{4h+4}) > \mathcal{E}(C_{4h}) - \mathcal{E}(P_{4h}).$$

Thus,

$$\mathcal{E}(C_{4h}) - \mathcal{E}(P_{4h}) > \mathcal{E}(C_8) - \mathcal{E}(P_8) \approx 9.65685 - 9.51754 = 0.139313 > 0. ▯$$

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