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On Energy of Trees with Perfect Matching

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Abstract

The energy of a graph is the sum of the absolute values of the eigenvalues of its adjacency matrix. We prove that the energy of a tree on n vertices with a perfect matching and maximum degree at most 3 is greater than $1.21n - 3.23$. This improves some known bounds on the energy of trees.

1 Introduction

1.1 Basics

Let G be a graph. Throughout this paper the *order* of G is the number of vertices of G. All the graphs that we consider are finite, undirected and simple. If $\{v_1, \ldots, v_n\}$ is the set of vertices of G, then the *adjacency matrix* of G, $A(G) = [a_{ij}]$, is an $n \times n$ matrix, where $a_{ij} = 1$ if v_i and v_j are adjacent and $a_{ij} = 0$ otherwise. Thus $A(G)$ is a symmetric matrix with zeros on the diagonal, and all eigenvalues of $A(G)$ are real. By eigenvalues of G we mean those of $A(G)$. We denote the *path* and the *star* graphs of order n by P_n and S_n, respectively. A *matching* of G is a set of mutually non-incident edges. A *perfect matching* of G is a matching which covers all vertices of G. The maximum degree of the vertices of G is denoted by $\Delta(G)$.

The *Hückel molecular orbital*, HMO theory, is nowadays on of the most important field of theoretical chemistry where graph eigenvalues occur. HMO theory deals with unsaturated conjugated molecules. The vertices of the graph associated with a given molecule are in one to one correspondence with the carbon atoms of the hydrocarbon system. Hückel theory in quantum chemistry insures that the total π-electron energy of a conjugated hydrocarbon is simply the energy of the corresponding molecular graph. The *energy* of a graph G (first introduced by Gutman [4]) is defined the sum of the absolute values of all eigenvalues of G and denoted by $E(G)$. For a survey on the energy of graphs, we refer the reader to the book [8] and the article [6].

1.2 Energy of Trees

Among n-vertex trees, the star S_n and the path P_n have, respectively, the minimum and maximum energy [3].

For integers $n \geq 3$ and $2 \leq k \leq n-1$, we denote by $P_{n,k}$ the *comet* of order n with k pendent vertices which is the tree formed by identifying an end vertex of the path P_{n-k+1} with the central vertex of the star S_k. In [11] it is proved that for any tree T of order n with k pendent vertices, $E(T) \geq E(P_{n,k})$, with equality holding if and only if T is isomorphic to $P_{n,k}$.

For chemical trees (i.e., trees with $\Delta(T) \leq 3$) Nikiforov [9] conjectured that there is a constant c such that for any $\epsilon > 0$, if T is a tree with large enough order n and $\Delta(T) \leq 3$, then $E(T) \geq (c - \epsilon)n$. Li and Liu [7] proved this conjecture.

A graph on n vertices, whose energy is less than n is called *hypoenergetic*. Graphs for which $E(G) \geq n$ are said to be *non-hypoenergetic*. It is known that (see [1] and [8, Theorem 9.1]) if the graph G is nonsingular (i.e., no eigenvalue of G is equal to zero), then G is non-hypoenergetic.

From the Sachs Theorem on the determinant of the adjacency matrices of graphs ([2, Theorem 1.3]) it follows that trees with a perfect matching are nonsingular. Therefore, trees having a perfect matching are *non-hypoenergetic*. As the main result of this paper, we improve this result by the following theorem.

Theorem 1. *Let T be tree on n vertices with a perfect matching and maximum degree at most* 3. *Then* $E(T) > 1.21n - 3.23$.

2 Proof of Theorem 1

For even n, the *comb graph* of order n, denoted by $\widehat{P}_{n/2}$, is a tree obtained by adding a pendent edge to each vertex of the path $P_{n/2}$ (see Figure 1).

We will need the following result of Zhang and Li [12] who confirmed a conjecture by Gutman [5].

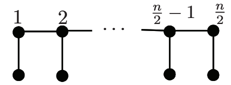

Figure 1. The comb graph $\widehat{P}_{n/2}$

Lemma 1. *Among trees on n vertices with a perfect matching and maximum degree at most 3, the energy is minimized by the comb graph $\widehat{P}_{n/2}$.*

Proof of Theorem 1. Let T be tree on n vertices with a perfect matching and $\Delta(T) \leq 3$. Since T has a perfect matching, it has an even number of vertices. So let $n = 2k$. By Lemma 1, $E(T) \geq E(\widehat{P}_k)$. So it is enough to prove the assertion for $\widehat{P}_k$. For the adjacency matrix of $\widehat{P}_k$, we have

$$A(\widehat{P}_k) = \begin{bmatrix} A(P_k) & I \\ I & O \end{bmatrix}.$$

By using the Schur complement (see [2, Lemma 2.2]),

$$\begin{aligned} \det(xI - A(\widehat{P}_k)) &= \det(xI - A(P_k)) \det(xI - (xI - A(P_k))^{-1}) \\ &= \det(x(xI - A(P_k)) - I) = x^k \det(\tfrac{x^2-1}{x} I - A(P_k)). \end{aligned}$$

It follows that if λ is an eigenvalue of P_k, then $\frac{1}{2}(\lambda \pm \sqrt{\lambda^2+4})$ is an eigenvalue of $\widehat{P}_k$. We know that the eigenvalues of P_k are

$$2\cos\left(\frac{\pi r}{k+1}\right), \quad r = 1, \ldots, k.$$

Therefore, the eigenvalues of $\widehat{P}_k$ are

$$\cos\left(\frac{\pi r}{k+1}\right) \pm \sqrt{1 + \cos^2\left(\frac{\pi r}{k+1}\right)}, \quad r = 1, \ldots, k.$$

It turns out that

$$E(\widehat{P}_k) = \sum_{r=1}^{k} 2\sqrt{1 + \cos^2\left(\frac{\pi r}{k+1}\right)} = 4 \sum_{r=1}^{\lfloor k/2 \rfloor} \sqrt{1 + \cos^2\left(\frac{\pi r}{k+1}\right)}\,.$$

By considering the upper Riemann sum (see [10, Section 3.2]) and since the cosine function is decreasing on the interval $[0, \pi/2]$, we have

$$\frac{\pi}{k+1} \sum_{r=0}^{\lfloor k/2 \rfloor} \sqrt{1 + \cos^2\left(\frac{\pi r}{k+1}\right)} > \int_0^{\pi/2} \sqrt{1 + \cos^2(x)} dx > 1.91.$$

It follows that

$$\sum_{r=1}^{\lfloor k/2 \rfloor} \sqrt{1 + \cos^2\left(\frac{\pi r}{k+1}\right)} > \frac{1.91(k+1)}{\pi} - \sqrt{2}\,.$$

Therefore

$$E(\widehat{P}_k) > \frac{4 \cdot 1.91(k+1)}{\pi} - 4\sqrt{2} = \frac{2 \cdot 1.91}{\pi} n + 4\left(\frac{1.91}{\pi} - \sqrt{2}\right) > 1.21n - 3.23\,,$$

which completes the proof of Theorem 1. ■

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