Linear Algebra and its Applications 453 (2014) 141–153

Contents lists available at ScienceDirect

Linear Algebra and its Applications

www.elsevier.com/locate/laa

On the minimal energy of graphs ☆

Jianbin Zhang [a,b,*], Haibin Kan [a]

[a] Shanghai Key Laboratory of Intelligent Information Processing, School of Computer Science, Fudan University, Shanghai 200433, China
[b] School of Mathematics, South China Normal University, Guangzhou 510631, China

ARTICLE INFO

Article history:
Received 15 March 2014
Accepted 6 April 2014
Available online 25 April 2014
Submitted by M. Benzi

MSC:
05C35
05C50
05C90

Keywords:
Minimal energy
Eigenvalue
Quasi-tree

ABSTRACT

The energy of a graph is the sum of the absolute values of the eigenvalues of the graph which is used to approximate the total π-electron energy of the molecule. In this paper, we determine the (n, e)-graphs with minimal energy for $e = n+1$ and $n+2$, which is giving a complete solution to the conjecture for $e = n + 1$ and $e = n + 2$ proposed by Caporossi et al. in [4]. Moreover, we determine the graphs with the minimal and second-minimal energies for $n - 1 \leq e \leq \frac{3n}{2} - 3$, and the unique graph with minimal energy for $\frac{3n-5}{2} \leq e \leq 2n - 4$ among all quasi-trees with n vertices and e edges, respectively.

☆ This work was supported by China Postdoctoral Science Foundation funded project (Grants No. 2012M520815 and No. 2013T60411), the National Natural Science Foundation of China (Grants No. 11001089 and No. 61170208), Shanghai Key Program of Basic Research (Grant No. 12JC1401400).
* Corresponding author.
E-mail addresses: zhangjb@scnu.edu.cn (J. Zhang), hbkan@fudan.edu.cn (H. Kan).

http://dx.doi.org/10.1016/j.laa.2014.04.009
0024-3795/

1. Introduction

Let G be a simple graph with n vertices. The energy of G was first defined by Gutman in 1978 as the sum of the absolute values of the eigenvalues of G [6]:

$$E(G)=\sum_{i=0}^{n}\left|\lambda_i(G)\right|,$$

where $\lambda_1(G),\lambda_2(G),\dots,\lambda_n(G)$ are the eigenvalues of G.

Let $A(G)$ be the adjacency matrix of G, $\phi(G,\lambda)=\sum_{i=0}^{n}a_i\lambda^{n-i}$ be the characteristic polynomial of $A(G)$. Then $E(G)$ can be also expressed as the Coulson integral formula [8]

$$E(G)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{x^2}\ln\left[\left(\sum_{i=0}^{\lfloor n/2\rfloor}(-1)^i a_{2i}x^{2i}\right)^2+\left(\sum_{i=0}^{\lfloor n/2\rfloor}(-1)^i a_{2i+1}x^{2i+1}\right)^2\right]dx. \qquad (1)$$

Since the energy of a graph can be used to approximate the total π-electron energy of the molecule, it has been intensively studied by some researchers (see [4,6,9,12,13,15,16,19–22]). For details and an overview of the results on graph energy, we refer to the recent book by Li, Shi, and Gutman [3] or the review papers [5,7].

A connected graph with n vertices and e edges is called an (n,e)-graph. We call an (n,e)-graph a unicyclic graph, a bicyclic graph and a tricyclic graph if $e=n,n+1$ and $n+2$, respectively. A graph G is called a quasi-tree, if there exists a vertex $w\in V(G)$ such that $G-w$ is a tree. Let $S_{n,e}$ be the graph obtained by the star S_n with $e-n+1$ additional edges all connected to the same vertex, and $B_{n,e}$ be the bipartite (n,e)-graph with two vertices on one side, one of which is connected to all vertices on the other side.

Many results on the minimal energy have been obtained for various classes of graphs. In [4], Caporossi et al. posed the following conjecture:

Conjecture 1. *Among all connected graphs G with $n\ge 6$ vertices and $n-1\le e\le 2(n-2)$ edges, the graph with minimum energy is $S_{n,e}$ for $e\le n+\lfloor (n-7)/2\rfloor$, and $B_{n,e}$ otherwise.*

In [4], they also confirmed the conjecture for $e=n-1$ and $e=2(n-2)$. Li et al. [14] showed that $B_{n,e}$ is the unique bipartite graph with minimal energy for $e\le 2n-4$. Hou confirmed the conjecture for $e=n$ [9] and showed that $S_{n,n+1}$ is the unique bicyclic graph with minimal energy among all n-vertex connected bicyclic graphs with at most one odd cycle [10]. Zhang and Zhou [11], Li et al. [17] partially solved Conjecture 1 for $e=n+1$ and $e=n+2$, respectively. For all graphs G on n vertices and e edges which contain no disjoint odd cycles of lengths k and l with $k+l\equiv 2 \pmod 4$, Zhang and Zhou [11] showed that $S_{n,n+1}$ is the unique bicyclic graph with minimal energy, and Li et al. [17] proved that $S_{n,n+2}$ is the unique tricyclic graph with minimal energy, respectively.