Applied Mathematics and Computation 296 (2017) 233–238

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Some new lower bounds for energy of graphs

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ARTICLE INFO

MSC:
05C50

Keywords:
Eigenvalue
Energy
Non-singular graphs
Adjacency matrix

ABSTRACT

The energy of a graph G, denoted by $\mathcal{E}(G)$, is defined as the sum of the absolute values of all eigenvalues of G. In this paper we present some new lower bounds for energy of non-singular graphs, connected non-singular graphs and connected unicyclic non-singular graphs in terms of number of vertices, number of edges, maximum degree and Zagreb indices.

1. Introduction

Let $G=(V,E)$ be a simple undirected graph with n vertices and m edges. We use $V(G)=\{v_1,v_2,\dots,v_n\}$, for $v_i\in V(G)$, the degree of v_i, written by $d(v_i)$ or d_i, is the number of edges incident with v_i. The *maximum vertex degree* is denoted by Δ. The *first* and *second Zagreb* indices are defined as $M_1(G)=\sum_{u\in V}d_u^2$ and $M_2(G)=\sum_{uv\in V}d_u d_v$. Two surveys of properties of M_1 and M_2 are found in [14]. Let $u,v\in V$, a *walk* of G from u to v is a finite alternating sequence $v_0(=u)e_1v_1e_2\dots v_{k1}e_kv_k(=v)$ of vertices and edges such that $e_i=v_{i-1}v_i$ for $i=1,2,\dots,k$. The number k is the length of the walk. In particular, if the vertex $v_i, i=0,1,\dots,k$, in the *walk* are all distinct then the walk is called a *path*, the *path graph* n vertices denoted by P_n. A *closed path* or *cycle*, is a path $v_1,\dots,v_k$ (where $k\geq 3$) together with the edge v_1v_k, the *cycle* graph n vertices denoted by C_n. If each pair of vertices in a graph is joined by a walk, the graph is said to be *connected*. A simple undirected graph in which every pair of distinct vertices is connected by a unique edge, is the *complete* graph and is denoted by K_n. In this paper we use the following usual notation. By n and m we denote the numbers of vertices and edges, respectively, of the underlying graph G. The *adjacency matrix* $A(G)$ of G is defined by its entries as $a_{ij}=1$ if $v_iv_j\in E(G)$ and 0 otherwise. The *eigenvalues* of graph G are the *eigenvalues* of its *adjacency matrix* $A(G)$, denoted by $\lambda_1\geqslant\lambda_2\geqslant\dots\geqslant\lambda_n$, where $n=|V(G)|$. The *spectral radius* of G, denoted by $\lambda_1(G)$, is the largest eigenvalue of $A(G)$. When more than one graphs are under consideration, then we write $\lambda_i(G)$ instead of λ_i. As well known,

$$detA=\prod_{i=1}^{n}\lambda_i.$$

A graph G is said to be *singular* if at least one of its *eigenvalues* is equal to zero. For *singular* graphs, evidently, $detA=0$. A graph is *non-singular* if all its *eigenvalues* are different from zero. Then, $|detA|>0$.

The *energy* of the graph G is defined as:

$$\mathcal{E}=\mathcal{E}(G)=\sum_{i=1}^{n}|\lambda_i|. \tag{1}$$

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http://dx.doi.org/10.1016/j.amc.2016.10.019
0096-3003/

This concept was introduced by Gutman and is intensively studied in chemistry, since it can be used to approximate the total π-*electron* energy of a *molecule* (see, [12,13]). This *spectrum-based* graph invariant has been much studied in both *chemical* and mathematical literature. Among the pioneering results of the theory of graph energy are the lower and upper bounds for energy (see [1,3,8,19]). For more information about energy of graph (see [4,9,10,15,18]).

McClellands lower bound for energy [17] depends on the parameters n, m, and $detA$, and reads:

$$\mathcal{E}(G) \geqslant \sqrt{2m + n(n-1) \mid detA \mid^{\frac{2}{n}}}. \tag{2}$$

It holds for all graphs. In particular, it holds for both singular and non-singular graphs. Caporossi et al. [2] discovered the following simple lower bound: let G be a graph with m edges. Then

$$\mathcal{E}(G) \geqslant 2\sqrt{m}, \tag{3}$$

with equality if and only if G is a complete bipartite graph plus arbitrarily many isolated vertices.

Das et al. lower bound for energy [7] depends on the parameters n, m, and $detA$, and reads:

$$\mathcal{E}(G) \geqslant \frac{2m}{n} + (n-1) + ln \mid detA \mid - ln\frac{2m}{n}. \tag{4}$$

In the section, we present some new lower bounds for energy of non-singular graphs, connected non-singular graphs and connected unicyclic non-singular graph in terms of number of vertices, number of edges, maximum degree and Zagreb indices.

2. Lemmas

We list here some previously known results that will be needed in the sections.

Lemma 1 [11]. *Let G be a non-empty graph with maximum vertex degrees* Δ. *Then*

$$\lambda_1 \geqslant \sqrt{\Delta}, \tag{5}$$

equality holds if and only if G is $\frac{n}{2}K_2$.

Lemma 2 [11]. *If G is a graph with n vertices, m edges, and degree sequence* $d_1, d_2, \ldots, d_n$, *then*

$$\lambda_1 \geqslant \frac{1}{m}\sum_{ij\in E}\sqrt{d_i d_j} = \frac{\sqrt{M_2}}{m}. \tag{6}$$

Lemma 3 [6]. *G has only one distinct eigenvalue if and only if G is an empty graph. G has two distinct eigenvalues* $\mu_1 > \mu_2$ *with multiplicities* m_1 *and* m_2 *if and only if G is the direct sum of* m_1 *complete graphs of order* $\mu_1 + 1$. *In this case,* $\mu_2 = -1$ *and* $m_2 = m_1\mu_1$.

Lemma 4 (Hong [16]). *If G is a connected unicyclic graph, then*

$$\lambda_1 \geq 2, \tag{7}$$

with equality if and only if G is a cycle C_n.

Lemma 5 (Collatz and Sinogowitz [5]). *If G is a connected graph with n vertices, then*

$$\lambda_1 \geq 2\cos\left(\frac{\pi}{(n+1)}\right), \tag{8}$$

with equality if and only if G is a cycle P_n.

Lemma 6 ([2]). *Let G be a graph with m edges. Then*

$$\mathcal{E}(G) \geqslant 2\sqrt{m}, \tag{9}$$

with equality if and only if G is a complete bipartite graph plus arbitrarily many isolated vertices.

3. Lower bounds for energy of non-singular graphs

In this section we obtain lower bounds for energy of non-singular graphs.

Theorem 1. *Let G be a non-empty and non-singular graphs with n vertices, m edge. Then*

$$\mathcal{E}(G) \geqslant \sqrt{\Delta} + (n-1) + ln \mid detA \mid - ln(\sqrt{\Delta}), \tag{10}$$

Equality holds in (10) if and only if $G \cong K_2$.