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Lower bounds for the energy of graphs

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Abstract

Let G be a finite simple undirected graph with n vertices and m edges. The energy of a graph G, denoted by $\mathcal{E}(G)$, is defined as the sum of the absolute values of the eigenvalues of G. In this paper we present lower bounds for $\mathcal{E}(G)$ in terms of number of vertices, edges, Randić index, minimum degree, diameter, walk and determinant of the adjacency matrix. Also we show our lower bound in (11) under certain conditions is better than the classical bounds given in Caporossi et al. (1999), Das (2013) and McClelland (1971).

Keywords: Energy (of non-singular graph); Determinant of adjacency matrix; Randić index; Spectral radius

1. Introduction

Let $G = (V, E)$ be a simple undirected graph with n vertices and m edges. 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 $distance$ between two vertices x and y, denoted by $d(x, y)$, is the number of edges of a $shortest\ path$ between x and y, and its $maximum$ value over all pair of vertices is called $diameter$ of the graph G, $\big(D = diam(G) = max\{d(x, y) :\ x, y \in V\}\big)$. The $minimum\ degree$ vertices of G, is denoted by $\delta(G)$. The *Randić index* of G, denoted by $R(G)$, is defined as $R = R(G) = \sum_{uv\in E} \frac{1}{\sqrt{d(v)d(u)}}$. A $walk$ of G from u to v is a finite alternating sequence $v_0(= u)e_1v_1e_2 \ldots v_{k1}e_kv_k(= v)$ of vertices and edges such that $e_i = v_{i-1}v_i$ for $i = 1, 2, \ldots, k$. The number k is the length of the $walk$. In particular, if the vertices v_i, $i = 0, 1, \ldots, k$, in the $walk$ are all distinct then the walk is called a $path$. The number of $walks$ of length k of G starting at v is denoted by $d_k(v)$. Clearly, one has $d_0(v) = 1$, $d_1(v) = d(v)$ and $d_{k+1}(v) = \sum_{w\in N(v)} d_k(w)$, where $N(v)$ is the set of all neighbors of the vertex v. 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 denoted by K_n. 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. Let $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n$ denote the $eigenvalues$ of $A(G)$. The $spectral\ radius$ of G, denoted by $\lambda_1(G)$,

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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 $non\text{-}singular$ if all its $eigenvalues$ are different from zero. Then, $\mid detA \mid > 0$. The $energy$ of the graph G is defined as

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

where λ_i, $i = 1, 2, \ldots, n$, are the $eigenvalues$ of graph G.
This concept was introduced by $Gutman$ and is intensively studied in $chemistry$, since it can be used to approximate the total $\pi\text{-}electron\ energy$ of a $molecule$ (see, e.g.[1,2]). This $spectrum\text{-}based$ graph invariant has been much studied in both $chemical$ and $mathematical$ literature. For details and an exhaustive list of references see the $monograph$ [3]. What nowadays is referred to as graph $energy$, defined via Eq. (1), is closely related to the total $\pi\text{-}electron$ energy calculated within the $Huckelmolecular$ orbital approximation; for details see [4,5]. Among the pioneering results of the theory of graph energy are the lower and upper bounds for $\mathcal{E}$, discovered by McClelland [11]. Has been much studied energy in the $Chemical$ and $Mathematics$ see [5–11].

$McClelland$ [12] obtained the following lower bound in terms of n, m and the $determinant$ of the $adjacency\ matrix$:

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

It holds for all graphs. In particular, it holds for both $singular$ and $non\text{-}singular$ graph.

In the $monograph$ [13] the following simple lower bound in terms of m is mentioned:

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

with equality holding if and only if G consists of a $complete\ bipartite$ graph $K_{a,b}$ such that $a \cdot b = m$ and arbitrarily many isolated vertices.
Recently, $Kinkar\ Ch.\ Das\ et\ al.$ [14] have given the following lower bound, valid for $non\text{-}singular$ graph:

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

The paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we present lower bounds on the energy $\mathcal{E}(G)$. In Section 4, we show our lower bound in (11) under certain conditions is better than the classical bounds given in [12–14].

2. Preliminaries

In this section, we shall list some previously known results that will be needed in the next two sections.

Lemma 1 ([15]). *Let G be a connected graph with m edges, n vertices. Then*

$$\lambda_1 \geqslant \frac{2m}{n}, \tag{5}$$

with equality if and only if G is a regular graph.

Lemma 2 ([16]). *Let G be a non-trivial graph with n vertices. Then*

$$R(G) \leqslant \frac{n}{2}. \tag{6}$$

Lemma 3 ([15]). *Let G be a connected graph with degree sequence $d_1, d_2, \ldots, d_n$. Then*

$$\lambda_1 \geqslant \frac{m}{R}. \tag{7}$$