Communications in Mathematical and in Computer Chemistry

Upper Bounds for the Energy of Graphs

Kinkar Ch. Das, Seyed A. Mojallal

Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea e-mail: kinkardas2003@googlemail.com e-mail: ahmad_mojalal@yahoo.com

(Received June 2, 2013)

Abstract

The energy of a graph G, denoted by E(G), is defined as the sum of the absolute values of all eigenvalues of G. In this paper we present some new upper bounds for E(G) in terms of number of vertices, number of edges, clique number, minimum degree, and the first Zagreb index.

1 Introduction

Let G = (V, E) be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set E(G), |E(G)| = m. Let d_i be the degree of the vertex v_i for $i = 1, 2, \ldots, n$. The maximum and minimum vertex degrees are denoted by Δ and δ , respectively. Let N_i be the neighbor set of the vertex $v_i \in V$. Denote by ω the clique number of the graph G. If the vertices v_i and v_j are adjacent, we denote this by $v_i v_j \in E(G)$. The adjacency matrix A(G) of G is defined by its entries as $a_{ij} = 1$ if $v_i v_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n$ denote the eigenvalues of A(G). λ_1 is called the spectral radius of the graph G. When more than one graphs are under consideration, then we write $\lambda_i(G)$ instead of λ_i .

Some well known results on graph eigenvalues are the following:

$$\sum_{i=1}^n \lambda_i = 0 \qquad , \qquad \sum_{i=1}^n {\lambda_i}^2 = 2m \ .$$

For more details see the monograph [1].

The energy of the graph G is defined as

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

For more details on the theory of graph energy see the monograph [3].

The paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we obtain two new upper bounds on energy E(G) of the graph G.

2 Preliminaries

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

Lemma 2.1. [6] Let B be a $p \times p$ symmetric matrix and let B_k be its leading $k \times k$ submatrix; that is, B_k is matrix obtained from B by deleting its last p - k rows and columns. Then for i = 1, 2, ..., k

$$\rho_{p-i+1}(B) \le \rho_{k-i+1}(B_k) \le \rho_{k-i+1}(B)$$

where $\rho_i(B)$ is the *i*-th largest eigenvalue of *B*.

Lemma 2.2. [5] Let
$$\mathbf{F} = \left\{ X = (x_1, x_2, \dots, x_n) : x_i \ge 0, \sum_{i=1}^n x_i = 1 \right\}$$
. Then
 $1 - \frac{1}{\omega(G)} = \max_{X \in \mathbf{F}} \langle X, AX \rangle$.

Lemma 2.3. (Schur's lemma [5]) For each rectangular array $\{c_{jk} : 1 \le j \le m, 1 \le k \le n\}$ and each pair of sequences $\{x_j : 1 \le j \le m\}$ and $\{y_k : 1 \le k \le n\}$,

$$\left|\sum_{j=1}^{m} \sum_{k=1}^{n} c_{jk} x_j y_k\right| \le \sqrt{RC} \left(\sum_{j=1}^{m} |x_j|^2\right)^{1/2} \left(\sum_{k=1}^{n} |y_k|^2\right)^{1/2}$$

where R and C are the row sum and column sum maxima defined by

$$R = \max_{j} \sum_{k=1}^{n} |c_{jk}|$$
 and $C = \max_{k} \sum_{j=1}^{m} |c_{jk}|$.

3 Upper bound on energy of graphs

In this section we give two upper bounds on energy . First we mention three earlier known such bounds. McClelland's famous bound is [4] $E \leq \sqrt{2mn}$. It was improved by Koolen and Moulton [2]:

$$E(G) \le \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}.$$
(1)

Zhou [7] obtained an upper bound

$$E(G) \le \sqrt{\frac{M_1}{n}} + \sqrt{(n-1)\left(2m - \frac{M_1}{n}\right)} \tag{2}$$

where M_1 stands for the first Zagreb index.

We are now ready to give an upper bound on energy in terms of n, m, δ , and ω .

Theorem 3.1. Let G be a graph of order n, with m edges, with minimum degree δ , and clique number ω . Then

$$E(G) \le \sqrt{2m(n-\delta) + 4\sqrt{m^3(1-1/\omega)}}$$
 (3)

Proof: First we have to prove that

$$\sum_{v_j v_k \notin E(G)} |\lambda_j \lambda_k| \le (n - 1 - \delta)m .$$
(4)

Putting $c_{jk} = a_{jk}(G^c)$, $x_j = |\lambda_j|$ and $y_k = |\lambda_k|$, in Lemma 2.3, we get

$$\sum_{j=1}^{n} \sum_{k=1}^{n} a_{jk}(G^c) |\lambda_j| |\lambda_k| \le \Delta(G^c) \sqrt{2m} \sqrt{2m} \quad \text{as} \quad \sum_{j=1}^{n} \lambda_j^2 = 2m$$

that is,

$$2\sum_{v_jv_k\notin E(G)}|\lambda_j||\lambda_k| \le (n-1-\delta)2m$$

which gives the result in (4).

Next we have to prove that

$$\sum_{v_j v_k \in E(G)} |\lambda_j \lambda_k| \le \sqrt{4m^3(1 - 1/\omega)} .$$
(5)

Putting $X = \frac{1}{2m}(\lambda_1^2, \ldots, \lambda_n^2)$ in Lemma 2.2, we have

$$1 - 1/\omega \ge \frac{1}{4m^2} \sum_{v_j v_k \in E(G)} \lambda_j^2 \lambda_k^2 \; .$$

-660-

By the Cauchy-Schwarz inequality and using the above result, we get

$$\frac{1}{m} \left(\sum_{v_j v_k \in E(G)} |\lambda_j \lambda_k| \right)^2 \le \sum_{v_j v_k \in E(G)} (\lambda_j \lambda_k)^2 \le 4m^2 (1 - 1/\omega)$$

that is,

$$\left(\sum_{v_j v_k \in E(G)} |\lambda_j \lambda_k|\right)^2 \le 4m^3(1 - 1/\omega)$$

which gives the result in (5).

Now,

$$\left(\sum_{i=1}^{n} |\lambda_i|\right)^2 = \sum_{i=1}^{n} \lambda_i^2 + 2\sum_{1 \le j < k \le n} |\lambda_j \lambda_k|,$$

that is,

$$E^{2} = 2m + 2 \sum_{v_{j}v_{k} \in E(G)} |\lambda_{j} \lambda_{k}| + 2 \sum_{v_{j}v_{k} \notin E(G)} |\lambda_{j} \lambda_{k}|$$

$$\leq 2m + 4\sqrt{m^{3}(1 - 1/\omega)} + 2m(n - 1 - \delta) \text{ by (4) and (5).}$$

This completes the proof.

Theorem 3.2. Let G be a connected graph of order $n \ (n \ge 6)$, with m edges, and with minimum degree δ . Then

$$E(G) \le \frac{2(m-\delta)}{n-1} + \sqrt{(n-1)\left[2m - \frac{4(m-\delta)^2}{(n-1)^2}\right]}.$$
(6)

Proof: First we have to prove that

$$\lambda_1(G) \ge \frac{2(m-\delta)}{n-1}$$

By Lemma 2.1,

$$\lambda_1(G) \ge \lambda_1(G')$$

where $\lambda_1(G') = \lambda_1(A_{n-1})$ and A_{n-1} is the leading $(n-1) \times (n-1)$ submatrix of A(G), obtained from A(G) by deleting its last row and column corresponding minimum degree vertex of degree δ . Thus we have

$$\lambda_1(G) \ge \lambda_1(G') \ge \frac{2m'}{n'} = \frac{2(m-\delta)}{n-1} \tag{7}$$

where m' and n' are the number of edges and the number of vertices in G', respectively.

Claim 1. For $n \ge 6$,

$$\frac{2(m-\delta)}{n-1} \ge \sqrt{\frac{2m}{n}} \,. \tag{8}$$

Proof of Claim 1: We have to prove that

$$\frac{(m-\delta)^2}{m} \ge \frac{(n-1)^2}{2n}$$

that is,

$$m - 2\delta + \frac{\delta^2}{m} \ge \frac{n}{2} - 1 + \frac{1}{2n}$$

that is,

$$2m - 4\delta \ge n - 2 + \frac{1}{n} - \frac{2\delta^2}{m} .$$

$$\tag{9}$$

For $\delta = 1$, one can easily see that the result in (9) holds as $m \ge n - 1$ and $n \ge 6$. Otherwise. $\delta \ge 2$. We now assume that $d_1 \ge d_2 \ge \cdots \ge d_n$. Thus we have

$$2m - 4\delta \ge \sum_{i=1}^{n-4} d_i \ge 2(n-4) \ge n - 2 + \frac{1}{n} - \frac{2\delta^2}{m}$$
 as $n \ge 6$

By the Cauchy–Schwarz inequality,

$$E(G) \le \lambda_1 + \sqrt{(n-1)(2m-\lambda_1^2)} .$$

One can see easily that

$$f(x) = x + \sqrt{(n-1)(2m-x^2)}$$

is a decreasing function on $\left(\sqrt{\frac{2m}{n}}, \sqrt{2m}\right)$. By Claim 1,

$$\sqrt{\frac{2m}{n}} \le \frac{2(m-\delta)}{n-1} \le \lambda_1(G)$$
.

From the above, we get

$$E(G) \le \frac{2(m-\delta)}{n-1} + \sqrt{(n-1)\left[2m - \frac{4(m-\delta)^2}{(n-1)^2}\right]}.$$

Corollary 3.3. Let G be a connected graph of order $n \ (n \ge 6)$, with m edges, and with at least a pendent vertex. Then

$$E(G) \le \frac{2(m-1)}{n-1} + \sqrt{(n-1)\left[2m - \frac{4(m-1)^2}{(n-1)^2}\right]} .$$
(10)

Proof: Since G has a pendent vertex, according to Theorem 3.2, we get

$$\lambda_1(G) \ge \frac{2(m-1)}{n-1}$$

and hence the result (10).

Remark 3.4. Our result (6) is better than (1) for

$$\frac{2(m-\delta)}{n-1} \ge \frac{2m}{n}$$

that is,

 $m \geq n \delta$.

Remark 3.5. Our result (6) is better than (2) for

$$\frac{2(m-\delta)}{n-1} \ge \sqrt{\frac{M_1(G)}{n}}$$

that is, if the condition $4n(m-\delta)^2 \ge M_1(G)(n-1)^2$ is obeyed. In particular, (6) is better than (2) for the complete graph K_{n-1} to which a pendent edge is attached.

Acknowledgement. This work is supported by the Faculty research Fund, Sungkyunkwan University, 2012.

References

- D. M. Cvetković, M. Doob, H. Sachs, Spectra of Graphs Theory and Application, Academic Press, New York, 1980.
- [2] J. H. Koolen, V. Moulton, Maximal energy graphs, Adv. Appl. Math. 26 (2001) 47–52.
- [3] X. Li, Y. She, I. Gutman, *Graph Energy*, Springer, New York, 2012.
- [4] B. J. McClelland, Properties of the latent roots of a matrix: The estimation of π-electron energies, J. Chem. Phys. 54 (1971) 640–643.
- [5] T. Motzkin, E. G. Straus, Maxima for graphs and a new proof of a theorem of Turán, Canad. J. Math. 17 (1965) 533–540.
- [6] J. R. Schott, Matrix Analysis for Statistics, Wiley, New York, 1997.
- [7] B. Zhou, Energy of graphs, MATCH Commun. Math. Comput. Chem. 51 (2004) 111–118.