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ON SPECTRAL MOMENTS AND ENERGY OF GRAPHS

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Abstract

Let G be a graph on n vertices, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues. The energy of G is $E = \sum_{i=1}^{n} |\lambda_i|$. The k-th spectral moment of G is $M_k = \sum_{i=1}^{n} (\lambda_i)^k$. We prove that for even positive integers r, s, t, such that $4r = s + t + 2$, the inequality $E \geq (M_r)^2/\sqrt{M_s\, M_t}$ holds for all graphs with at least one edge, thus generalizing an earlier result [de la Peña, Mendoza, Rada, *Discr. Math.* **302** (2005) 77–84]. The graphs for which the above relation becomes equality are characterized.

INTRODUCTION

Let G be a graph without loops and multiple edges. Let n and m be, respectively, the number of vertices and edges of G. The eigenvalues of G are denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, and are assumed to be labelled in a non-increasing manner:

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \ .$$

The basic properties of graph eigenvalues can be found in the book [1].

The *energy* of the graph G is defined as

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

The graph–energy concept has a chemical motivation. Namely, for graphs which in the Hückel molecular orbital theory represent the carbon–atom skeleton of some conjugated hydrocarbons, E is related to the total π-electron energy (or more precisely: the total π-electron energy is a linear function of E). For more details on this matter see the book [2] and the recent review [3].

However, more than a quarter of century ago, one of the present authors proposed [4] that the graph invariant E — as defined above — be considered for all graphs, irrespective of its possible chemical interpretation. This change of viewpoint made it possible to envisage and establish numerous new, generally valid, mathematical properties of E, some of evident value for chemistry, some of no visible chemical applicability.

After 1978 the graph–energy concept was presented to the mathematico–chemical community on several other occasions [2, 5, 6]. Initially, the response of other colleagues was almost nil. However, around the turn of the century the study of E suddenly became a rather popular topic both in mathematical chemistry and in "pure" mathematics. Of the numerous papers on graph energy that recently appeared, we quote here only a few [7–29].

For a nonnegative integer k, the k-th *spectral moment* of the graph G is defined as

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k \ . \tag{2}$$

Note that M_k is equal to the number of closed walks of length k in G [1].

Because both the energy and the spectral moments are symmetric functions of graph eigenvalues, it is reasonable to ask if there exist relations between them. Much work has been devoted to problems of this kind [30–39].

Recently, de la Peña et al. [25] proved the following:

Theorem 1. *Let G be a bipartite graph with at least one edge and let r , s , t be even positive integers, such that $4r = s + t + 2$. Then*

$$E(G) \geq M_r(G)^2 \; [M_s(G) \, M_t(G)]^{-1/2} \quad . \tag{3}$$

In this article we show that the statement of Theorem 1 can be, in a natural manner, extended to all graphs, and also offer a simple proof of the inequality Eq. (3).

EXTENDING THEOREM 1

In Eq. (3) it is essential that the parameters s and t are (non-negative) even integers, because in the case of bipartite graphs, the odd spectral moments are necessarily zero [1]. In order to overcome this limitation we define the moment–like quantities

$$M_k^* = M_k^*(G) = \sum_{i=1}^{n} |\lambda_i|^k \quad . \tag{4}$$

Here k may be an odd integer, but also any real–valued number. Comparing Eqs. (2) and (4) we conclude that if k is an even integer, then $M_k^* = M_k$. Bearing in mind (1), we see that $M_1^* = E$.

The main result of this section is the following extension of Theorem 1:

Theorem 1a. *Let G be a graph with at least one edge and let r , s , t be non-negative real numbers, such that $4r = s + t + 2$. Then*

$$E(G) \geq M_r^*(G)^2 \, [M_s^*(G) \, M_t^*(G)]^{-1/2} \quad . \tag{5}$$

Evidently, Theorem 1 is a special case of Theorem 1a for G being a bipartite graph and for s and t being even positive integers.

In order to prove Theorem 1a we need a simple lemma.

Lemma 2. *Let $a_1, a_2, \ldots, a_h$ be positive real numbers, $h > 1$, and let r, s, t be non-negative real numbers, such that $4r = s + t + 2$. Then*

$$\left[\sum_{i=1}^{h} (a_i)^r\right]^4 \leq \left(\sum_{i=1}^{h} a_i\right)^2 \sum_{i=1}^{h} (a_i)^s \sum_{i=1}^{h} (a_i)^t \,. \tag{6}$$

If $(s,t) \neq (1,1)$, then the equality in (6) holds if and only if $a_1 = a_2 = \cdots = a_h$.

Note that if $s = t = 1$ (and, consequently, $r = 1$), then equality in (6) holds in a trivial manner for any choice of a_i's.

Proof. By the Cauchy–Schwarz inequality,

$$\begin{aligned} \left[\sum_{i=1}^{h} (a_i)^r\right]^4 &= \left[\sum_{i=1}^{h} (a_i)^{(s+t)/4} \cdot (a_i)^{1/2}\right]^4 \leq \left[\sum_{i=1}^{h} (a_i)^{(s+t)/2} \sum_{i=1}^{h} a_i\right]^2 \\ &= \left[\sum_{i=1}^{h} (a_i)^{s/2} \cdot (a_i)^{t/2}\right]^2 \left[\sum_{i=1}^{h} a_i\right]^2 \leq \sum_{i=1}^{h} (a_i)^s \sum_{i=1}^{h} (a_i)^t \left(\sum_{i=1}^{h} a_i\right)^2 . \end{aligned}$$

This proves (6). Equality in (6) holds if and only if both a_i^{s+t-2} and a_i^{s-t} are constant for all $i = 1, 2, \ldots, h$. Thus if $(s,t) \neq (1,1)$, then equality in (6) holds if and only if $a_1 = a_2 = \cdots = a_h$. $\square$

Proof of Theorem 1a. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_h$ be the non-zero eigenvalues of the graph G. Since G has at least one edge, we have [1] $\mu_1 = \lambda_1 > 0$ and $\mu_h = \lambda_n < 0$.

Using Lemma 2 for the positive numbers $a_i = |\mu_i|$, $i = 1, 2, \ldots, h$, and noting that in this case $\sum_{i=1}^{h} (a_i)^k = M_k^*(G)$ and, in particular, $\sum_{i=1}^{h} a_i = E(G)$, we have

$$M_r^*(G)^4 \leq E(G)^2 \, M_s^*(G) \, M_t^*(G)$$

from which (5) follows. $\square$

If $s = t = 1$, then in a trivial manner (5) becomes an equality. By Lemma 2, if $(s,t) \neq (1,1)$, then equality in (5) holds if and only if $|\mu_1| = |\mu_2| = \cdots = |\mu_h|$. We now determine the graphs that obey these conditions.

Theorem 3. *Equality in (5) holds if and only if the components of the graph G are isolated vertices and/or complete bipartite graphs $K_{p_1,q_1},\ldots,K_{p_k,q_k}$ for some $k \geq 1$, such that $p_1\,q_1 = \cdots = p_k\,q_k$.*

Proof. If G is a graph specified in the theorem with $p_i\,q_i = C$ for $i = 1,\ldots,k$, it is easy to check [1] that its non-zero eigenvalues are $\sqrt{C}$ (k times) and $-\sqrt{C}$ (k times), and so the equality in (5) holds.

Suppose that the equality in (5) holds. Then $|\mu_1| = |\mu_2| = \cdots = |\mu_h|$. Note that, by Theorem 0.13 in [1], it must be $\sum_{i=1}^{h} \mu_i = 0$. Therefore the spectrum of G must be symmetric w. r. t. the origin, and thus (by Theorem 3.11 in [1]), G is a bipartite graph. Note also that G has either two (μ_1 and $-\mu_1$) or three (μ_1, $-\mu_1$, and 0) distinct eigenvalues. Then by Theorems 6.4 and 6.5 in [1], G is the disjoint union of complete bipartite graphs $K_{p_1,q_1},\ldots,K_{p_k,q_k}$ for some $k \geq 1$, such that $p_1\,q_1 = \cdots = p_k\,q_k$, and possibly isolated vertices. $\square$

DISCUSSION

By setting $(s,t) = (0,2)$ in Theorem 1a (which implies $r = 1$), we obtain $E \leq \sqrt{2m(n-n_0)}$ where n_0 is the number of zero eigenvalues of the underlying graph. This improvement of the famous McClelland upper bound $E \leq \sqrt{2mn}$ [2, 3] seems to be first reported in [40].

By setting $(s,t) = (2,4)$ in Theorem 1a (which implies $r = 2$), we obtain the lower bound

$$E \geq 2\sqrt{2}\,m\sqrt{\frac{m}{M_4}}\ .$$

For bipartite graphs it has been reported in [13, 25], whereas for all (both bipartite and non-bipartite) graphs in [16, 41].

* * * * *

The relation $4r = s+t+2$ used in Lemma 2 may be viewed as a special case of

$$2^k\,r = s+t+2^k-2 \tag{7}$$

for $k = 2$. With condition (7), with $k \geq 2$ and k integer, instead of (6) we get

$$\left[\sum_{i=1}^{h}(a_i)^r\right]^{2^k} \leq \left(\sum_{i=1}^{h} a_i\right)^{2^k-2} \sum_{i=1}^{h}(a_i)^s \sum_{i=1}^{h}(a_i)^t \ .$$

which, in turn, implies

$$E(G) \geq M_r^*(G)^{2^k/(2^k-2)} \left[M_s^*(G)\, M_t^*(G)\right]^{-1/(2^k-2)} \ .$$

The condition $4r = s + t + 2$ can be further modified. For instance, if $8r = s + t + u + 5$, then

$$\left[\sum_{i=1}^{h}(a_i)^r\right]^{8} \leq \left(\sum_{i=1}^{h} a_i\right)^{5} \sum_{i=1}^{h}(a_i)^s \sum_{i=1}^{h}(a_i)^t \sum_{i=1}^{h}(a_i)^u$$

and

$$E(G) \geq M_r^*(G)^{8/5} \left[M_s^*(G)\, M_t^*(G)\, M_u^*(G)\right]^{-1/5} \ .$$

If $8r = s + t + u + v + 4$, then

$$\left[\sum_{i=1}^{h}(a_i)^r\right]^{8} \leq \left(\sum_{i=1}^{h} a_i\right)^{4} \sum_{i=1}^{h}(a_i)^s \sum_{i=1}^{h}(a_i)^t \sum_{i=1}^{h}(a_i)^u \sum_{i=1}^{h}(a_i)^v$$

and

$$E(G) \geq M_r^*(G)^{2} \left[M_s^*(G)\, M_t^*(G)\, M_u^*(G)\, M_v^*(G)\right]^{-1/4} \ .$$

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