MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **91** (2024) 797–803
ISSN: 0340–6253
doi: 10.46793/match.91-3.797G

Note on Some New (n, m)-Type Bounds for Graph Energy

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(Received December 28, 2023)

Abstract

The classical results by McClelland (1971) and Koolen & Moluton (2001) provide upper bounds for graph energy in terms of number of vertices (n) and number of edges (m). Recently, in *MATCH Commun. Math. Comput. Chem.* **79** (2018) and **91** (2024), new such (n, m)-type bounds were communicated. In this paper, we analyze these bounds and find that one is identical to the Koolen–Moulton bound, whereas the other is inferior to it.

1 Introduction

Throughout this paper G denotes a simple connected graph possessing n vertices and m edges. The energy of G, denoted by $\mathcal{E}(G)$, is the sum of absolute values of the eigenvalues of the adjacency matrix of G. Details and additional references on the mathematical theory of graph energy can be found in the book [8], whereas on its chemical origin and applications in the book [5] and the survey [4].

One of the earliest results on graph energy is the (n, m)-type upper bound

$$\mathcal{E}(G) \leq \sqrt{2mn}$$

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discovered in 1971 by McClelland [9]. Thirty years later, Koolen and Moulton succeeded to find a better such bound [6], namely

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

For bipartite graphs, the above bound can be additionally sharpened as [7]:

$$\mathcal{E}(G) \leq \frac{4m}{n} + \sqrt{(n-2)\left[2m - 2\left(\frac{2m}{n}\right)^2\right]}\,. \tag{2}$$

Until quite recently, these were the only known (n, m)-type upper bounds for graph energy [8]. Few years ago, in the paper [1], a new such bound was reported, namely:

$$\mathcal{E}(G) \leq 2 + \sqrt{(n-1)(2m-4)} \tag{3}$$

which (according to [1]) would hold only for connected unicyclic graphs. Eventually, the same group of authors [2], extended Eq. (3) to all connected graphs, except trees, as:

$$\mathcal{E}(G) \leq 2k + \sqrt{(n-1)(2n+2k-6)} \tag{4}$$

where $k = m - n + 1$ is the cyclomatic number of G (= number of independent cycles); $k = 1$ for unicyclic graphs, $k = 2$ for bicyclic graphs, etc. In [2], it was assumed that $k \geq 1$, i.e., trees ($k = 0$) were excluded.

In what follows, we examine the inequalities (3) and (4) and establish a number of their weak points.

2 Unicyclic graphs, $k = 1$

For connected unicyclic graphs, $m = n$. If we take this condition into account, then Eq. (1), after a minute calculation, reduces to Eq. (3). Thus we arrive at:

Observation 1. *Eq. (3) is identical to the Koolen–Moulton bound, as applied to unicyclic graphs.*

It is really surprising that the authors of [1] did not notice the above fact. Not only that they quote the paper [6], but (correctly) state the Koolen–Moulton bound (i.e., Eq. (1)) on the bottom of page 288. (On the next page, they also state Eq. (2), incorrectly.)

For the authors' comfort: The bound (3), when applied to connected unicyclic graphs, is correct.

3 Polycyclic graphs, $k \geq 2$

If $k \geq 2$, then it is easy to show that the right-hand side of (4) is greater than the right-hand side of (1). Note first that

$$\frac{2m}{n} = 2 + 2\,\frac{k-1}{n}\,.$$

For $k = 2, 3, 4, 5, 6, 7$, the value of n is at least 4,4,5,5,5,6, respectively. Then by direct checking we get

$$2 + 2\,\frac{k-1}{n} < 2k\,. \tag{5}$$

For larger values of n, the validity of (5) is evident.

Next,

$$\begin{aligned} 2m - 2\left(\frac{2m}{n}\right)^2 &= 2n + 2k - 2 - \left(2 + 2\,\frac{k-1}{n}\right)^2 \\ &= 2n + 2k - 6 - 8\,\frac{k-1}{n} - 4\left(\frac{k-1}{n}\right)^2 \end{aligned}$$

and therefore

$$2m - 2\left(\frac{2m}{n}\right)^2 < 2n + 2k - 6\,. \tag{6}$$

Bearing in mind the inequalities (5) and (6), we conclude that

$$\frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} < 2k + \sqrt{(n-1)(2n+2k-6)}$$

holds for all values of m and n that graphs with $k \geq 2$ may have. This leads to:

Observation 2. *For all connected polycyclic graphs ($k \geq 2$), the upper bound Eq. (4) for graph energy is weaker than the Koolen–Moulton bound, Eq. (1).*

In other words, the (n,m)-type upper bound Eq. (4), reported in [2], is valueless.

Although the expression in Eq. (3) was claimed to hold only for $k = 1$, we could try to apply it also for larger values of k. By numerical testing we arrived at:

Observation 3. *For all connected polycyclic graphs ($k \geq 2$), the upper bound Eq. (3) for graph energy is weaker than the Koolen–Moulton bound, Eq. (1).*

4 Trees, $k = 0$

In both papers [1] and [2], it was indicated that the inequalities (3) and (4) do not hold for $k = 0$, i.e., cannot be applied to trees. Nevertheless, we checked these inequalities also for trees, and obtained somewhat unexpected results.

Trees are bipartite graphs. Therefore, for estimating the energy of trees, also Eq. (2) may be applied (which necessarily gives better results than Eq. (1)).

In Table 1 are presented the results of Eqs. (1)–(4), calculated for n-vertex trees.

Among n-vertex trees, the path P_n has the greatest energy [3]. Therefore, for comparative purposes, in Table 1 also the $\mathcal{E}(P_n)$-values are included.

n	$\mathcal{E}(P_n)$	Eq. (1)	Eq. (2)	Eq. (3)	Eq. (4)
2	2.0000	2.0000	2.0000	–	–
3	2.8284	3.4415	3.3333	*2.0000*	*0.0000*
4	4.4721	4.8541	4.7321	*4.4495*	*2.4495*
5	5.4641	6.2648	6.1394	**6.0000**	*4.0000*
6	6.9879	7.6759	7.5497	**7.4772**	*5.4772*
7	8.0547	9.0877	8.9614	**8.9282**	*6.9282*
8	9.5175	10.5000	10.3739	**10.3666**	*8.3666*
9	10.6275	11.9127	11.7868	11.7980	*9.7980*
10	12.0533	13.3256	13.2000	13.2250	*11.2250*
11	13.1915	14.7388	14.6134	14.6491	*12.6491*
12	14.5925	16.1521	16.0270	16.0712	*14.0712*
13	15.7505	17.5656	17.4407	17.4919	*15.4919*
14	17.1335	18.9792	18.8544	18.9115	*16.9115*
15	18.3063	20.3928	20.2683	20.3303	**18.3303**
16	19.6759	21.8065	21.6822	21.7484	**19.7484**
17	20.8601	23.2203	23.0961	23.1660	**21.1660**
18	22.2191	24.6341	24.5101	24.5832	**22.5832**
19	23.4124	26.0480	25.9240	26.0000	**24.0000**
20	24.7630	27.4619	27.3381	27.4165	**25.4165**
21	25.9637	28.8758	29.7521	28.8328	**26.8328**
22	27.3073	30.2898	30.1661	30.2489	**28.2489**
23	28.5141	31.7037	31.5802	31.6648	**29.6648**
24	29.8519	33.1177	32.9943	33.0805	**31.0805**
25	31.0639	34.5318	34.4084	34.4962	**32.4962**

Table 1. Results of Eqs. (1)–(4), applied to n-vertex trees, compared to the energy of the respective path, $\mathcal{E}(P_n)$. For some values of n, Eqs. (3) and (4) produce impossible values, smaller than $\mathcal{E}(P_n)$; these are indicated by italics. For some values of n, Eqs. (3) and (4) yield upper bounds for energy better than Koolen–Moulton's; these are indicated by boldface.

Our calculations point out a remarkable feature of Eq. (4):

Observation 4. *For sufficiently large values of n (in fact, for $n \geq 15$), the upper bound Eq. (4) for the energy of trees is sharper than the Koolen–Moulton bounds, Eqs. (1) and (2).*

When considering (m,n)-type upper bounds for the energy of trees, one must note that the best such bond is [8]

$$\mathcal{E}(G) \leq \mathcal{E}(P_n) = \begin{cases} \dfrac{2}{\sin \frac{\pi}{2(n+1)}} - 2 & \text{if } n \text{ is even} \\ \\ \dfrac{2 \cos \frac{\pi}{2(n+1)}}{\sin \frac{\pi}{2(n+1)}} - 2 & \text{if } n \text{ is odd.} \end{cases} \tag{7}$$

Therefore, in the case of trees, the quest for other such bounds happens to be to a great deal pointless.

5 Concluding remarks

The present analysis shows that the (n,m)-type upper bounds for graph energy, reported in [1,2], either duplicate an earlier known result (in case of unicyclic graphs) or are inferior to earlier known results (in case of bicyclic, tricyclic, tetracyclic, ..., graphs). Only in the case of trees, for sufficiently large values of n, the bound (4) slightly outruns those by Koolen and Moulton, Eqs. (1) and (2), but – of course – is weaker than the bound (7).

Therefore, as before, the Koolen–Moulton estimates (1) and (2) remain the best known (n,m)-type upper bounds for graph energy.

***Acknowledgment*:** Izudin Redžepović acknowledges financial support from the Serbian Ministry of Science, Technological Development, and Innovation (Grant No. 451-03-47/2023-01/200122) and the State University of Novi Pazar.

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