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ON BORDERENERGETIC GRAPHS

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A b s t r a c t. A graph G of order n is said to be borderenergetic if its energy is equal to $2n - 2$ and if $G \ncong K_n$. The first such graph was discovered in 2001, but their systematic study started only in 2015. The main hitherto established results on borderenergetic graphs are outlined, and a few new established. Borderenergetic graphs (of the same order) are mutually equienergetic. The difference in their structure indicates which structural features of a graph can vary, without affecting the value of its energy. In particular, it is shown that this applies to the number of edges.

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1. *Introduction*

Let G be a simple graph of order n, possessing m edges. Let the eigenvalues of G (i.e., the eigenvalues of the adjacency matrix of G) be $\lambda_1, \lambda_2, \ldots, \lambda_n$ [5]. The energy of the graph G is defined as

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

This graph–spectrum–based invariant has been extensively studied. Details of its mathematical theory can be found in [28] whereas details of its chemical applications in [21].

The upper bound

$$\mathcal{E} \leq \sqrt{2mn}$$

was established by McClelland in the early 1970s [32]. In the same paper [32], an approximate formula was proposed:

$$\mathcal{E} \approx a\sqrt{2mn} \quad , \quad a \approx 0.9 \tag{1.1}$$

which was eventually demonstrated to be highly accurate in the case of molecular graphs [14, 22]. An additional corroboration of this formula was the analogous lower bound

$$\mathcal{E} \geq \sqrt{\frac{16}{27}}\sqrt{2mn}$$

that holds for certain molecular graphs, in particular, for hexagonal systems [12].

According to formula (1.1), the energy of a graph would be a monotonically increasing function of the number m of edges. If this formula could be applied to all graphs, then among graphs with a fixed number n of vertices, the complete graph K_n would have the greatest energy, equal to $\mathcal{E}(K_n) = 2n - 2$. Counterexamples for this naive conjecture were soon discovered [4]. Somewhat later [38], the first systematic construction of graphs with the property $\mathcal{E}(G) > \mathcal{E}(K_n)$ were reported.

Graphs of order n with the property $\mathcal{E}(G) > 2n - 2$ were named *hyperenergetic* [15]. Numerous classes of hyperenergetic graphs have been recognized; for details see the survey [18], and the recent paper [9]. The search for hyperenergetic graphs became purposeless after Nikiforov proved in 2007 [33] that for almost all n-vertex graphs

$$\mathcal{E} = \left(\frac{4}{3\pi} + o(n)\right) n^{3/2}$$

implying that almost all graphs are hyperenergetic.

The question that remained open was if there exist graphs of order n, other than K_n, satisfying the equality

$$\mathcal{E}(G) = 2n - 2\,.$$

In 2015, such graphs were named *borderenergetic* [11]. It is understood that the complete graph is not borderenergetic.

2. *Existence and Properties of Borderenergetic Graphs*

The first borderenergetic graph was discovered by Yaoping Hou and the present author already in 2001 [24], but in that time it failed to attract any attention. This

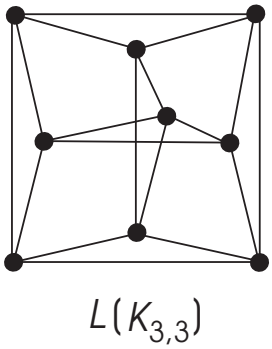

Figure 1. The first borderenergetic graph, discovered in year 2001

borderenergetic graph is the line graph of the complete bipartite graph $K_{3,3}$, depicted in Fig. 1. It has 9 vertices and its spectrum is

$$Sp(L(K_{3,3}) = \{4, 1, 1, 1, 1, -2, -2, -2, -2\}\,.$$

Therefore, $\mathcal{E}(L(K_{3,3})) = 16 = 2 \cdot 9 - 2 = \mathcal{E}(K_9)$.

The first systematic research of borderenergetic graphs is reported in the paper [11], which was then continued in [7, 10, 25, 29, 30, 34]. By means of computer-aided checking, the following was established.

Theorem 2.1. 1° *There are no borderenergetic graphs of order* $n \leq 6$ [11].

2° *There exists a borderenergetic graph* G_0 *of order* 7*, depicted in Fig.* 2*. Its spectrum is:*

$$Sp(G_0) = \{5, 1, -1, -1, -1, -1, -2\}\,.$$

This graph is unique [11].

3° *For any* $n \geq 7$*, there exist borderenergetic graphs of order* n [11].

4° *There are exactly* 6 *borderenergetic graphs of order* 8 [11].

5° *There are exactly* 17 *borderenergetic graphs of order* 9 [11].

6° *Finding the* 10*-vertex borderenergetic graphs was a less easy task. After some mistakes* [29]*, the exact value was determined to be* 49 [34].

7° *There are exactly* 158 *borderenergetic graphs of order* 11. [34]. *Of these,* 157 *are connected* [10].

A graph is said to be integral if all its eigenvalues are integers [5]. The energy of an integral graph is necessarily an integer. (As shown in [2], if $\mathcal{E}$ is integer, then it

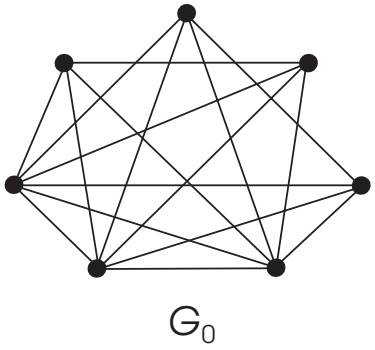

Figure 2. The smallest borderenergetic graph, $n = 7$, $\mathcal{E}(G_0) = 12$

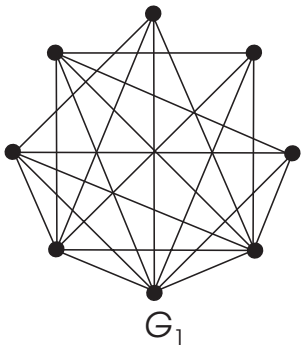

Figure 3. One of the three distinct non-integral borderenergetic graphs of smallest order, $n = 8$, $\mathcal{E}(G_1) = 14$

must be even.) Before the discovery of borderenergetic graphs, all known graphs with integer energy were integral, and the following conjecture seemed to be plausible:

Conjecture 2.1. *If $\mathcal{E}(G)$ is an integer, then the graph G is integral.*

Conjecture 2.1 is false. Some borderenergetic graphs provide counterexamples for it. A simple such example is the graph G_1 of order 8, depicted in Fig. 3. Its spectrum is

$$Sp(G_1) = \left\{3 + \sqrt{6}, 1, 3 - \sqrt{6}, -1, -1, -1, -2, -2\right\} .$$

Two graphs G_a and G_b are said to be *equienergetic* if $\mathcal{E}(G_a) = \mathcal{E}(G_b)$ [1, 3]. In a trivial manner, cospectral graphs are equienergetic. However, there exist numerous

pairs, triplets, and larger families of mutually non-cospectral graphs that are equienergetic [28]. Evidently, borderenergetic graphs of equal order are equienergetic. Thus, the results stated in Theorem 2.1 point out large families of mutually equienergetic graphs.

It is generally believed that the two main structural features of a graph that affect the values of its energy are the number of vertices n and the number of edges m (for details see [13, 16, 17] and the references quoted therein). This could be stated in the form of the following:

Empirical rule 2.1. (a) *If two graphs have equal number of vertices and equal number of edges, then their energies do not differ significantly.*

(b) *If two graphs of the same order are equienergetic, then the number of their edges do not differ significantly.*

The fact is that Rule 2.1 was tested and verified on countless examples [14, 22, 32], but only for molecular graphs. On the other hand, molecular graphs possess a relatively small number of edges, usually $m \leq \frac{3}{2}n$. From the study of borderenergetic graphs, it becomes evident that in the case of graphs with larger number of edges, Rule 2.1 could be drastically violated, especially its part (b).

Indeed, the number of edges in families of borderenergetic graphs vary significantly. For instance, the six borderenergetic graphs of order $n = 8$ have m-values between 19 and 25. Among the 158 borderenergetic graphs of order $n = 11$, there are graphs with m between 25 and 49. Moreover, m may assume any value in the mentioned interval, except $m = 42, 46, 48$ [34].

Theorem 2.2. *A borderenergetic graph of order n must possess at least $2n - 2$ edges.*

PROOF. We start with the Koolen–Moulton upper bound [26]:

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

In view of it, the value of m satisfying the equality

$$\frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} = 2n - 2 \tag{2.1}$$

such that $m \neq n(n-1)/2$, is a lower bound for the number of edges of a borderenergetic graph. For $n \geq 2$, (2.1) can be transformed into the quadratic equation

$$2m^2 - (n-1)(n+4)m + 2n(n-1)^2 = 0$$

whose solutions are $m = n(n-1)/2$ and $m = 2(n-1)$. Therefore, any borderenergetic graph must satisfy $m \geq 2(n-1)$. □

Theorem 2.3. *A bipartite borderenergetic graph of order n must possess at least $\lceil m_0 \rceil$ edges where*

$$m_0 = \frac{1}{8}\left(n^2 + 6n - 8 - \sqrt{n^4 - 20n^3 + 84n^2 - 128n + 64}\right). \qquad (2.2)$$

PROOF. We use an analogous reasoning as in the proof of Theorem 2.2, applying it to the Koolen–Moulton upper bound for bipartite (n, m)-graphs [27]:

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

It leads to the quadratic equation

$$4m^2 - (n^2 + 6n - 8)m + 2n(n-1)^2 = 0$$

whose smaller solution is the expression (2.2). □

Recall that for large values of n, m_0 is asymptotically equal to $\frac{16}{n}(n-1)^2$.

The bound $m \geq 2(n-1)$ in Theorem 2.2 is not the best possible. However, as seen from point 4 of the next Theorem 2.4, it is quite close to the optimal value.

Several general methods for constructing borderenergetic graphs have been elaborated [7, 11, 25]. Some of these are aimed at generating regular [7] or threshold borderenergetic graphs [25]. The following results were established for borderenergetic graphs with small maximal vertex degree Δ:

Theorem 2.4 ([30])**.** 1° *There are no borderenergetic graphs with $\Delta \leq 3$.*

2° *There are no borderenergetic graphs with $\Delta = 4$ of order greater than 21.*

3° *Borderenergetic graphs with $\Delta = 4$ are non-bipartite.*

4° *Borderenergetic graphs of order n with $\Delta = 4$ have either $2n$ or $2n-1$ edges.*

Corollary 2.1. *If $m = 2n$, then the borderenergetic graphs with $\Delta = 4$ are 4-regular. If $n = 2n - 1$, then the borderenergetic graphs with $\Delta = 4$ are either 4-regular with one edge deleted (i.e., with $n-2$ vertices of degree 4 and two vertices of degree 3) or 4-regular with an additional vertex of degree 2 (i.e., with $n-1$ vertices of degree 4 and one vertex of degree 2).*

Corollary 2.2. *The number of borderenergetic graphs with $\Delta = 4$ is finite.*

It would be interesting to construct all borderenergetic graphs with $\Delta = 4$, or – at least – to determine their number.

By means of an extensive computer search, the following was established.

Claim 2.1 ([10]). 1° *There are no borderenergetic graphs of order* $n \leq 8$ *and* $n = 10, 11, 12, 13, 14, 16, 17$ *for which* $\Delta = 4$.

2° *There exist two borderenergetic graphs of order* 9 *and one of order* 15 *for which* $\Delta = 4$.

3° *If there exist additional borderenergetic graphs with* $\Delta = 4$*, their order must be between* 18 *and* 21.

3. *Extensions*

The complete graph K_n is regular. Therefore, its Laplacian energy [23] coincides with the ordinary graph energy, $\mathcal{E}_L(K_n) = \mathcal{E}(K_n) = 2n - 2$. Bearing this in mind, one may seek for L-borderenergetic graphs, namely graphs different from K_n, satisfying the condition $\mathcal{E}_L(G) = 2n - 2$. Several recent papers are devoted to this topic [6, 8, 31, 35, 36, 37].

In addition to the ordinary graph energy $\mathcal{E}$ and the Laplacian energy $\mathcal{E}_L$, numerous other "graph energies" $\mathcal{E}_X$ have been considered in the last few years [19, 20]. Some of these "energies" have the property that for graphs with a fixed order n, $\mathcal{E}_X(K_n)$ is maximal. If this is not the case, then it would be possible to seek for X-borderenergetic graphs. In the present author's opinion, it is just a matter of time before papers on X-borderenergetic graphs will start to appear in the mathematical literature.

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