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Orderenergetic Graphs

Saieed Akbari[1,*], **Maryam Ghahremani**[2], **Ivan Gutman**[3], **Fatemah Koorepazan–Moftakhar**[1]

[1] *Department of Mathematical Sciences, Sharif University of Technology, Azadi Street, P.O. Box 11155-9415, Tehran, Iran*
s_akbari@sharif.edu , f.moftakhar@sharif.edu

[2] *Department of Mathematics, Azad University, Science and Researcher Branch Tehran, Iran*
maryam.ghahremanii14@gmail.com

[3] *Faculty of Science, University of Kragujevac, P.O.Box 60, 34000 Kragujevac, Serbia*
gutman@kg.ac.rs

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Abstract

A graph is said to be orderenergetic if its energy is equal to its order. It is shown that there are infinitely many connected orderenergetic graphs. Some basic properties of these graphs are established. Several open problems and conjectures are pointed out.

1 Introduction

Let $G = (\mathbf{V}, \mathbf{E})$ be a simple graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. Let the order $|\mathbf{V}(G)|$ and size $|\mathbf{E}(G)|$ of G be denoted by n and m, respectively. By $\lambda_1, \lambda_2, \ldots, \lambda_n$ are denoted the eigenvalues of the $(0,1)$-adjacency matrix of G. Then the energy of G is [14]

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

Graphs satisfying the condition $\mathcal{E}(G) < n$ were named *hypoenergetic* [10], and their properties were studied in due detail [7, 8, 10, 14, 15]. In the present paper we focus our

*Corresponding author

attention to graphs for which $\mathcal{E}(G) = n$, i.e., graphs whose energy and order are equal, and call them *orderenergetic graphs*.

As usual, by P_n, C_n, and $K_{n_1,\dots,n_k}$ we denote the path and cycle of order n, and the complete k-partite graph of order $n_1 + \cdots + n_k$.

The complete bipartite graph with $a+b$ vertices is denoted by $K_{a,b}$. If $a = b$, we say that $K_{a,b}$ is balanced. Since the order of $K_{a,a}$ is $2a$, and since [4]

$$Spec(K_{a,a}) = \{a, 0, 0, \cdots, 0, -a\}$$

implying $\mathcal{E}(K_{a,a}) = 2a$, it immediately follows that all balanced complete bipartite graphs are orderenergetic. It is therefore of interest to find other connected orderenergetic graphs.

In [15], it was conjectured that there are exactly four connected orderenergetic graphs with maximal vertex degree at most 3 (Conjecture 3.7 in [15]). These four graphs are $K_{1,1}$, $K_{2,2}$, $K_{3,3}$, and the 6-vertex tree depicted in Fig. 1. This conjecture was eventually confirmed by Li and Ma [13].

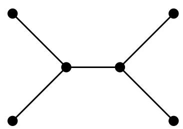

Figure 1: An orderenergetic graph of order 6.

Lemma 1. [3] *There are no connected orderenergetic graphs of odd order.*

By means of a computer-aided search, for connected graphs of even order up to 10, we established the following:

(i) If $n = 2$, the only connected orderenergetic graph is $K_{1,1} \cong P_2$.

(ii) If $n = 4$, the only connected orderenergetic graph is $K_{2,2} \cong C_4$.

(iii) If $n = 6$, there are two connected orderenergetic graphs: $K_{3,3}$ and the tree depicted in Fig. 1.

(iv) If $n = 8$, there are four connected orderenergetic graphs: $K_{4,4}$ and the graphs depicted in Fig. 2.

(v) If $n = 10$, the only connected orderenergetic graph is $K_{5,5}$.

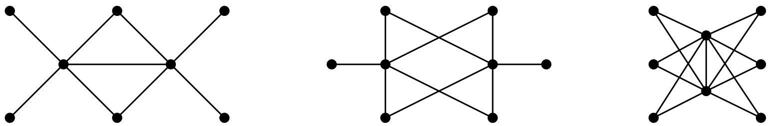

Figure 2: Orderenergetic graphs of order 8.

2 Constructing connected orderenergetic graphs

Lemma 2. [4] *The characteristic polynomial of the complete multipartite graph $K_{n_1,\dots,n_k}$ is*

$$\phi(K_{n_1,\dots,n_k}, x) = x^{n-k}\left(1-\sum_{i=1}^{k}\frac{n_i}{x+n_i}\right)\prod_{j=1}^{k}(x+n_j)\,.$$

Lemma 3. *For every positive integer p, the graph $K_{p,p,6p}$ is orderenergetic.*

Proof. By Lemma 2, $\phi(K_{p,p,6p}, x) = x^{8p-3}\,(x-4p)(x+p)(x+3p)$. Therefore $\mathcal{E}(K_{p,p,6p}) = 8p$. ■

Remark 4. *Based on a computer-aided search, it seems that $K_{p,p,6p}$ are the only orderenergetic complete multipartite graphs with at least 3 parts.*

Let G and H be two graphs of order n_G and n_H, respectively. Let $g, g' \in \mathbf{V}(G)$ and $h, h' \in \mathbf{V}(H)$. The direct product of G and H, denoted by $G \times H$, is a graph of order $n_G \cdot n_H$, whose vertex set is $\mathbf{V}(G) \times \mathbf{V}(H)$, and whose vertices (g, h) and (g', h') are adjacent if and only if $gg' \in \mathbf{E}(G)$ and $hh' \in \mathbf{E}(H)$ [12]. Thus,

$$\begin{aligned}\mathbf{V}(G\times H) &= \{(g,h) \mid g\in \mathbf{V}(G) \text{ and } h\in \mathbf{V}(H)\},\\ \mathbf{E}(G\times H) &= \{(g,h)(g',h') \mid gg'\in \mathbf{E}(G) \text{ and } hh'\in \mathbf{E}(H)\}.\end{aligned}$$

The direct product $G \times H$ is connected if and only if either G or H (or both) is non-bipartite. In addition, $G \times H$ is non-bipartite if and only if both G and H are non-bipartite [12].

If the eigenvalues of G are λ_i, $i = 1, 2, \dots, n_G$ and the eigenvalues of H are μ_j, $j = 1, 2, \dots, n_H$, then the spectrum of $G \times H$ consists of the products $\lambda_i \cdot \mu_j$, $i = 1, 2, \dots, n_G$, $j = 1, 2, \dots, n_H$ [4]. This immediately implies [17]

$$\mathcal{E}(G \times H) = \mathcal{E}(G) \cdot \mathcal{E}(H)\,.$$

Lemma 5. *If G and H are orderenergetic graphs, then also $G \times H$ is orderenergetic.*

Since we are interested in constructing connected orderenergetic graphs, we need to apply Lemma 5 to non-bipartite species. At this point one should observe that $K_{p,p,6p}$ as well as the left–hand side and the right–hand side graphs in Fig. 2 are non-bipartite.

Theorem 1. *There are infinitely many connected orderenergetic graphs, different from balanced complete bipartite graphs.*

Proof. First construction: If G_1 is a connected non-bipartite orderenergetic graph, then $G = G_1 \times G_1$ is also connected non-bipartite orderenergetic, as well as $G \times G_1$, etc. This construction can be continued infinitely many times.

Second construction: If G_1 and G_2 are two connected non-bipartite orderenergetic graphs, then $G = G_1 \times G_2$ is also connected non-bipartite orderenergetic, as well as $G \times G_1$ and $G \times G_2$, etc. This construction can be continued infinitely many times.

Third construction: If G_1 is a connected non-bipartite orderenergetic graph, and G_2 is a connected bipartite orderenergetic graph, then $G = G_1 \times G_2$ is connected bipartite orderenergetic, as well as $G_1 \times G$, etc. This construction can be continued infinitely many times. For G_2 we may use any balanced complete bipartite graph. ■

The graph $K_{p,p,6p}$ is non-bipartite, of order $8p$. At this moment we know of only two more non-bipartite orderenergetic graphs, both of order 8 (see Fig. 2). Bearing this in mind, we have:

Corollary 6. *There are connected orderenergetic graphs of order* $8p$, $p = 1, 2, \ldots$, *different from balanced complete bipartite graphs.*

3 Structural properties of orderenergetic graphs

In [1] a proof was presented of the von Neumann's trace inequality [11, p.458]. Based on it, in what follows we characterize the orderenergetic graphs having a $\{1, 2\}$-factor.

A $\{1, 2\}$-factor of a graph G is a spanning subgraph of G whose each component is P_2 or a cycle. In mathematical chemistry, $\{1, 2\}$-factors are usually referred to as Sachs graphs [5, 6, 9].

Theorem 2. *Let G be graph of order n. If G has a $\{1, 2\}$-factor, then $\mathcal{E}(G) \geq n$. Equality holds if and only if G is the disjoint union of balanced complete bipartite graphs.*

In order to prove Theorem 2, we need some preparations.

Lemma 7. [2] *Let G be a graph and $H_1, \ldots, H_k$ be its k vertex–disjoint induced subgraphs. Then*

$$\mathcal{E}(G) \geq \sum_{i=1}^{k} \mathcal{E}(H_i)\,.$$

Lemma 8. [1, Theorem 9.] *Let G be a graph of order n. If G has a $\{1,2\}$-factor, then $\mathcal{E}(G) \geq n$.*

A matching M in a graph G is a set of pairwise non-adjacent edges of G. A maximum matching is a matching that contains the largest possible number of edges. If a matching covers all vertices of G, then it is called a perfect matching. The matching number of G, denoted by $\mu(G)$, is the number of edges in a maximum matching.

Lemma 9. [18] *Let G be a bipartite graph. Then $\mathcal{E}(G) \geq 2\mu(G)$. Equality holds if and only if G is the disjoint union of balanced complete bipartite graphs and isolated vertices.*

Lemma 10. [1, Lemma 33.] *If $n \geq 10$, then $\mathcal{E}(C_n) \geq n+2$.*

Lemma 11. *If n is an odd integer, then $\mathcal{E}(C_n) > n$.*

Proof. If $n \geq 10$, then by Lemma 10, $\mathcal{E}(C_n) > n$. By direct computation, one gets $\mathcal{E}(C_3) = 4$, $\mathcal{E}(C_5) = 6.472$, $\mathcal{E}(C_7) = 8.988$ and $\mathcal{E}(C_9) = 11.517$, which completes the proof. ■

Proof of Theorem 2. It suffices to prove the theorem for connected graphs. Let a $\{1,2\}$-factor of G consists of cycles $C^{(1)}, \ldots, C^{(k)}$ and t copies of P_2. One may assume that every odd cycle in the $\{1,2\}$-factor is an induced odd cycle, because if we have an odd cycle with a chord, then there is a chord which partitions the vertices of odd cycle into an odd induced cycle and some paths of order 2. Now, by Lemma 7, we find that,

$$\mathcal{E}(G) \geq \sum_{i=1}^{k} \mathcal{E}(C^{(i)}) + t\,\mathcal{E}(P_2) = \sum_{i=1}^{k} \mathcal{E}(C^{(i)}) + 2t\,.$$

If at least one of the $C^{(i)}$ is an odd cycle, then by Lemma 7, $\mathcal{E}(G) > n$. So, let all $C^{(i)}$ be even. It follows that G has a perfect matching.

Now, by induction on the number of vertices, we prove that if $\mathcal{E}(G) = n$, then G is the disjoint union of balanced complete bipartite graphs.

For $n = 2$, the assertion holds. Let $n \geq 4$ and $M = \{u_1v_1, \ldots, u_{\frac{n}{2}}v_{\frac{n}{2}}\}$ be a perfect matching of G. Suppose that $H = G \setminus \{u_1, v_1\}$. Obviously, H has a perfect matching and so by Lemma 7, $\mathcal{E}(G) \geq \mathcal{E}(H) + 2$. If $\mathcal{E}(H) > n-2$, then $\mathcal{E}(G) > n$, a contradiction.

Thus assume that $\mathcal{E}(H) = n - 2$. By the induction hypothesis, every component of H is a balanced complete bipartite graph. Let $H_1, \ldots, H_r$ be the components of H.

If $r \geq 3$, then the induced subgraph on $(\bigcup_{i=2}^{r} \mathbf{V}(H_i)) \cup \{u_1, v_1\}$ is a connected graph and so by the induction hypothesis it is a complete bipartite graph, a contradiction.

Let $r = 1$ and $u_p v_p \in \mathbf{E}(H_1)$, $u_1 u_p \in \mathbf{E}(G)$. Now, for every i, $2 \leq i \leq p$, $i \neq p$, the induced subgraph on $\{u_1, u_p, u_i, v_1, v_p, v_i\}$ is a connected graph having a perfect matching. By the induction hypothesis, this subgraph is $K_{3,3}$ and so G is a balanced complete bipartite graph.

Suppose finally that $r = 2$. Assume that $u_p v_p \in \mathbf{E}(H_1)$ and $u_\ell v_\ell \in \mathbf{E}(H_2)$ and $N(u_p) \cap \{u_1, v_1\} \neq \emptyset$, $N(u_\ell) \cap \{u_1, v_1\} \neq \emptyset$. Since the induced subgraph on $\{u_1, u_p, u_\ell, v_1, v_p, v_\ell\}$ is connected and contains a perfect matching, by the induction hypothesis it is isomorphic to $K_{3,3}$, a contradiction.

The proof is thus complete. ■

Corollary 12. *A graph having a $\{1,2\}$-factor is orderenergetic if and only if it is the disjoint union of balanced complete bipartite graphs.*

A graph G is said to be non-singular if all its eigenvalues are different from zero. Otherwise, G is singular.

Theorem 3. *The only non-singular connected orderenergetic graph is $K_{1,1} \cong P_2$.*

Proof. For a graph G with n vertices, m edges and adjacency matrix $\mathbf{A}(G)$, the following lower bound for energy holds [14, 16]:

$$\mathcal{E}(G) \geq \sqrt{2m + n(n-1)|\det \mathbf{A}(G)|^{2/n}}\,.$$

If G is non-singular, then $|\det \mathbf{A}(G)| \geq 1$, and for such graphs

$$\mathcal{E}(G) \geq \sqrt{2m + n(n-1)}\,.$$

If, in addition, G is orderenergetic, then it must be

$$n \geq \sqrt{2m + n(n-1)}$$

from which it follows

$$\frac{2m}{n} \leq 1\,.$$

Since $2m/n$ is the average vertex degree, in case of connected graphs the latter condition is possible only if $2m/n = 1$ and then only for $G \cong P_2$. ■

The algebraic multiplicity of the number zero in the spectrum of a graph is referred to as its nullity, and is denoted by η.

Theorem 4. *There is no connected orderenergetic graph with $\eta = 1$.*

Proof. Let G be a connected orderenergetic graph of order n with nullity 1. By Lemma 1, n is even. Let the characteristic polynomial of G be $\phi(G, x) = \sum_{i=0}^{n} c_i \, x^{n-i}$. Since $\eta = 1$, it must be $c_n = 0$ and $c_{n-1} \neq 0$. Then by the Sachs theorem [5, 6, 9], G contains a $\{1, 2\}$-subgraph of order $n-1$, say H. Since H has odd order, it contains at least one odd cycle C. By Lemma 11 and noting that $\mathcal{E}(C_3) = 4$, $\mathcal{E}(C_5) = 6.472$, $\mathcal{E}(C_7) = 8.988$ and $\mathcal{E}(C_9) = 11.517$, we have $\mathcal{E}(C) > |\mathbf{V}(C)| + 0.2$.

Let $\mathbf{V}(G) \setminus \mathbf{V}(H) = \{w\}$. If the vertex w is adjacent to an odd cycle of G, then G has a $\{1, 2\}$-factor and so by Theorem 2, $G \cong K_{\frac{n}{2}, \frac{n}{2}}$, implying $\eta(G) = n - 2$, a contradiction.

One can assume that H has no even cycles, because the vertex set of every even cycle can be partitioned into disjoint copies of P_2.

Assume now that w is not adjacent to an odd cycle, and that it is adjacent to a vertex u_1, where $u_1 v_1$ is a component of H. Consider the induced subgraph on $\{w, u_1, v_1\}$, and call it L. Obviously, $\mathcal{E}(L) > |\mathbf{V}(L)| - 0.2$. By Lemma 7,

$$\mathcal{E}(G) \geq \mathcal{E}(L) + \mathcal{E}(C) + \mathcal{E}\big(G \setminus [\mathbf{V}(C) \cup \mathbf{V}(L)]\big) .$$

Since $G \setminus (\mathbf{V}(C) \cup \mathbf{V}(L))$ has a $\{1, 2\}$-factor, by Theorem 2, we conclude that

$$\mathcal{E}(G) > |\mathbf{V}(L)| + |\mathbf{V}(C)| + |\mathbf{V}\big(G \setminus [\mathbf{V}(C) \cup \mathbf{V}(L)]\big)| = n \, ,$$

a contradiction. ■

Remark 13. *As the proofs of Theorems 3 and 4 show, each connected graph with nullity at most 1 is non-hypoenergetic.*

4 Problems and conjectures

In [13] it was proven that among connected graphs whose vertex degrees are at most 3, there is a finite number (four) of orderenergetic species.

Conjecture 14. *Let $\Delta \geq 4$. The number of connected orderenergetic graphs, whose vertex degrees are at most Δ, is finite.*

Problem 15. *Verify Conjecture 14 for* $\Delta = 4$*. Find all corresponding graphs. This would be of particular value for chemical applications.*

Problem 16. *Verify Conjecture 14 for* $\Delta = 5$*,* $\Delta = 6$*, etc. Find all corresponding graphs.*

Our computational studies indicate that there are very few orderenergetic trees.

Problem 17. *Find a method for constructing orderenergetic trees.*

Conjecture 18. *There is a finite number of orderenergetic trees.*

In the proof of Theorem 1 we outlined methods for constructing connected orderenergetic graphs using the direct product of two graphs.

Problem 19. *Find a method for constructing connected orderenergetic graphs, not using the direct product.*

With regard to Corollary 6, we have:

Problem 20. *Find connected orderenergetic graphs (different from balanced complete bipartite graphs) of order* $8p+2$ *for some* p*. Same for* $8p+4$ *and* $8p+6$*.*

In Fig. 2 is depicted a bicyclic orderenergetic graph.

Problem 21. *Are there connected unicyclic orderenergetic graphs, other than* $K_{2,2}$ *?*

Conjecture 22. *For a given non-negative integer* k*, there are finitely many connected orderenergetic graphs with nullity* k*.*

Conjecture 23. *For a given non-negative integer* k*, there are finitely many connected hypoenergetic graphs with nullity* k*.*

In Theorems 2, 3, and 4 we established structural and spectral properties that orderenergetic graphs must (or must not) possess.

Problem 24. *Find more such properties.*

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