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HYPERENERGETIC LINE GRAPHS

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Abstract

If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of a graph G on n vertices, then the energy of this graphs is defined as $E(G) = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$. A graph is said to be hyperenergetic if $E(G) > 2n - 2$. It is shown that if G has more than $2n - 1$ edges, then its line graph is necessarily hyperenergetic. By this, a new method is acquired for constructing hyperenergetic graphs with any number of vertices (nine or more) and with relatively few edges.

INTRODUCTION

The concept of the energy of a graph has been described in due detail in a preceding paper [1] and elsewhere [2-4]. Thus if $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues [3, 5] of the graph G, then the *energy* of this graph is defined as

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

Details on the role of $E(G)$ in chemistry can be found in Chapter 12 of the book [3] and in the review [6].

Some time ago it was conjectured [2] that among all graphs on n vertices, the complete graph K_n has the greatest energy; $E(K_n) = 2n - 2$. Not long after that, it was recognized [7, 8] that the conjecture is false and that there exist graphs for which $E(G) > 2n - 2$. Graphs on n vertices, the energy of which exceeds $2n - 2$ are referred to as *hyperenergetic graphs*.

Fifteen years ago a computer-aided search [8] revealed that hyperenergetic graphs exist already for $n = 8$, but not for $n < 8$. However, the first systematic and general method for the construction of such graphs was put forward only recently by Walikar, Ramane and Hampiholi [9]. They demonstrated that the line graph $L(K_p)$ of the complete graph K_p was hyperenergetic for $p \geq 5$. By this, an infinite family of hyperenergetic graphs was obtained with $n = p(p-1)/2$, $p = 5, 6, 7, \ldots$ vertices. One of the present authors gave another general method for constructing hyperenergetic graphs by deleting a few edges from K_n [10, 11]. This construction furnishes hyperenergetic graphs for all $n \geq 9$. Subsequent computer studies [12] indicated that among graphs with large number of edges hyperenergetic species are encountered quite frequently. Anyway, all hyperenergetic graphs designed so far [9–13] have too many edges to be molecular graphs of conjugated π-electron systems, and should be viewed as graph representations of inorganic clusters, so called *cluster graphs* [14, 15]. The applicability of graph eigenvalues in the theory of clusters is long known [15].

In this paper we focus our attention to the energy of line graphs. Our main finding is that if a p-vertex graph G has more than $2p - 1$ edges, then its line graph $L(G)$ is necessarily hyperenergetic. Consequently, hyperenergetic graphs with relatively few edges can be constructed for all $n \geq 9$.

A CHEMICAL RATIONALE FOR STUDYING HYPERENERGETIC GRAPHS

The chemical applications of the total π-electron energy were outlined in the preceding paper [1]. In view of the importance of this quantity, it it not surprising that the question

how E depends on molecular structure?

was extensively studied. By possessing and answer to this question, at least a partial one, we would know something about the structural factors responsible for the stability of polycyclic conjugated molecules (which for a long time is known to be in a non-trivial manner related to the size and mutual arrangement of the cycles, on branching of the carbon atom skeleton, etc). What may be even more attractive to experimentalists, we would be able to predict which polycyclic conjugated molecules are "*aromatic*" and which are "*antiaromatic*", and to do this in an (at least rough) quantitative manner. This could then lead to the design of conjugated systems with non-standard (but desired) properties

In spite of enormous efforts in the past half a century, we are still pretty far from having a comprehensive and satisfactory answer to the above question. However, at this moment our ignorance is not complete (see, for instance, the review [6]).

The most obvious question one may ask about the structure-dependence of E is certainly

how E depends on molecular size?

Needless to say that the knowledge of the size-dependence of E is a prerequisite for any other study of the molecular structure-dependence of total π-electron energy.

Here under "molecular size" we understand the number of carbon atoms (n) and the number of carbon-carbon bonds (m). Recall that a conjugated hydrocarbon with parameters n and m has the constitutional formula C_nH_{3n-2m}. Consequently, all isomers have the same n and m values.

One of the results known since the 1970s [16] is that the E-value of conjugated molecules is (in the majority of cases, but not always) a monotonically increasing function of the parameters n and m, and that E is roughly proportional to $\sqrt{mn}$. This finding, however, could never been proven in a rigorous manner and could only be corroborated by statistical analysis.

Now, if $E \sim \sqrt{mn}$ would be applicable to all graphs, then, for a fixed value of n, the graph with maximal number of edges (= the complete graph K_n) would have the maximal energy. This reasoning is, in fact, the origin of the (false) conjecture [2]

mentioned in the previous section. In other words, if $E \sim \sqrt{mn}$ would be applicable to all graphs, then no hyperenergetic graphs would exist.

The existence of hyperenergetic graphs in a fully transparent manner demonstrates that the Ansatz $E \sim \sqrt{mn}$ is not generally applicable.

In order to try to save the $E \sim \sqrt{mn}$ approximation one may argue that *(i)* hyperenergetic graphs are just certain "pathological" cases, exceptions from the general rule and that their number is statistically insignificant. Further, hyperenergetic graphs might be "pathological" also in the sense that *(ii)* they contain too many edges to be chemically relevant. Alas, neither *(i)* nor *(ii)* is true, as we prove in this paper (cf. Theorem 1 below).

The fact that the line graphs of the majority of graphs are hyperenergetic has the following chemically important implication: In the general case, the actual size-dependence of the energy of a graph G, and therefore the actual molecular-size dependence of the total π-electron energy of a conjugated molecule, is somewhat more perplexed than suggested by the simple $\sqrt{mn}$ Ansatz.

It is believed that the study of hyperenergetic graphs sheds some more light on the structural features that influence the E-value (and therefore influence the stability of a conjugated molecule). Although it seems that no hyperenergetic graph is a genuine molecular graph (representing a chemically sound carbon-atom-based π-electron network), the conclusions obtained by the examination of the energies of such species could be directly applied in chemical considerations. Once we discover which exactly are the conditions for a graph to have maximal or nearly maximal energy, we will be able to pinpoint the details of molecular structure that may lead to the design of (from a practitioner's point of view) interesting and attractive conjugated π-electron systems. At this moment such conditions are not known. We nevertheless believe that the present research brings us a step closer to this ultimate goal.

LINE GRAPHS AND THEIR ENERGIES

We first fix our notation and terminology. A graph with p vertices and q edges will be referred to as a (p, q)-graph. Let G be a (p, q)-graph. Then the *line graph* [17]

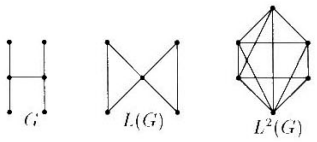

Fig. 1. A graph and its line graph

of G, denoted by $L(G)$, is the graph whose vertices are the edges of G. Two vertices of $L(G)$ are adjacent if the corresponding edges of G are incident. The number of vertices and edges of $L(G)$ will be denoted by n and m, respectively.

If the degrees of the vertices of G are $\delta_1, \delta_2, \ldots, \delta_p$, then, as well known [17],

$$n = q \quad ; \quad m = \frac{1}{2}\sum_{i=1}^{p} \delta_i^2 - q \,. \tag{1}$$

The line graph of $L(G)$ is denoted by $L^2(G)$. The higher iterated lines graphs are defined analogously: $L^3(G) = L(L^2(G))$, $L^4(G) = L(L^3(G))$, etc.

For further details on line graphs and iterated line graphs see [17]. A survey of the chemical applications of line graphs with an exhaustive bibliography is found in the introductory part of the paper [18]. An example is depicted in Fig. 1.

Let $A(G)$ and $A(L(G))$ be the adjacency matrices of the graphs G and $L(G)$, respectively. The $q \times p$ edge–vertex incidence matrix of the graph G, denoted by $R = ||r_{ij}||$, is defined via

$$r_{ij} = \begin{cases} 1 & \text{if the } i\text{-th edge and the } j\text{-th vertex are incident} \\ 0 & \text{otherwise} \,. \end{cases}$$

It is well known [5, 17] that the following relations are obeyed:

$$R^t R = D(G) + A(G) \tag{2}$$

$$R R^t = 2I + A(L(G)) \tag{3}$$

where I is the unit matrix of order n, R^t is the transpose of R, and $D(G) = \mathrm{diag}(\delta_1, \delta_2, \ldots, \delta_p)$.

From Eq. (2) we have that $D(G) + A(G)$ is a nonnegative-definite matrix and, consequently, its eigenvalues are all nonnegative. From Eqs. (2) and (3), and the fact that the matrices $R\,R^t$ and $R^t\,R$ have the same non-zero eigenvalues [5], we obtain

$$\phi(L(G)\,,\,\lambda) = (\lambda+2)^{q-p}\,\det[(\lambda+2)\,I - (D(G)+A(G))]$$

where $\phi(L(G)\,,\,\lambda)$ is the characteristic polynomial of $L(G)$. Therefore, if the eigenvalues of $D(G)+A(G)$ are $\mu_1 \le \mu_2 \le \cdots \le \mu_p$, then

$$\sum_{i=1}^{p} \mu_i = \sum_{i=1}^{p} \delta_i = 2\,q \tag{4}$$

and the eigenvalues of $L(G)$ are

$$-2 \ \ (\ q-p \text{ times}) \ \ ; \ \ \mu_i - 2\ ,\ i = 1,2,\ldots,p\ .$$

Hence, the energy of $L(G)$ satisfies the following relations:

$$\begin{aligned} E(L(G)) &= 2(q-p) + \sum_{i=1}^{p} |\mu_i - 2| \ge 2(q-p) + \sum_{i=1}^{p} (|\mu_i| - 2) \\ &= 2(q-p) + \sum_{i=1}^{p} (\mu_i - 2) = 2(q-p) + \sum_{i=1}^{p} \mu_i - 2p \end{aligned}$$

from which it follows

$$E(L(G)) \ge 4(q-p) \qquad \text{i. e.,} \qquad E(L(G)) \ge 2(q-1) + (2q-4p+2)\ . \tag{5}$$

From inequality (5) it is evident that if $2q - 4p + 2 > 0$, i. e., if $q \ge 2p$, then $E(L(G)) > 2(q-1)$.

Note that $q \le p(p-1)/2$. Therefore if $q \ge 2p$ then $p \ge 5$. We thus arrived at the main result of this paper:

Theorem 1. *Let $p \ge 5$ and let G be a (p,q)-graph. If $q \ge 2p$, then $L(G)$ is hyperenergetic.*

The line graph of the $(5,9)$-graph, obtained by deleting one edge from K_5, is hyperenergetic. On the other hand, there are no $(5,8)$-graphs whose line graphs are hyperenergetic. There are nine $(6,11)$-graphs, all having hyperenergetic line graphs.

Some examples of graphs having hyperenergetic line graphs are depicted in Fig. 2.

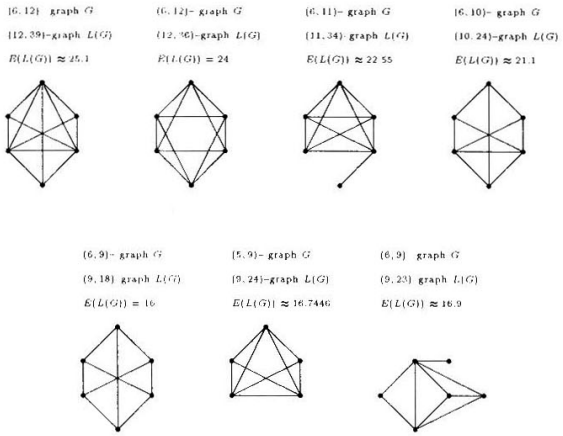

Fig. 2. Some graphs whose line graphs are hyperenergetic; note that for the first graph in the second row, $E(L(G)) = E(K_9)$ and thus the respective line graph is not strictly hyperenergetic

For any integer $n \geq 12$, there exists an integer $p \geq 6$, such that $2p \leq n \leq p(p-1)/2$. This implies:

Corollary 1.1. *By means of Theorem 1 it is possible to construct hyperenergetic graphs with n vertices for every $n \geq 9$.*

Let G be a (p, q)-graph with $q \geq 2p$. Then $L(G)$ is a hyperenergetic (n, m)-graph, with n, m conforming to Eqs. (1). Using the Cauchy–Schwarz inequality

$$\left(\sum_{i=1}^{N} a_i\, b_i\right)^2 \leq \sum_{i=1}^{N} a_i^2 \sum_{i=1}^{N} b_i^2\,,$$

choosing in it $N = p$, $a_i = \delta_i$ and $b_i = 1$, and bearing in mind Eqs. (1) and (4), we

arrive at

$$m = \frac{1}{2}\sum_{i=1}^{p} \delta_i^2 - q \geq \frac{1}{2}\,\frac{(2q)^2}{p} - q \geq 3q = 3n \ .$$

Since $L(G)$ has more than $2n$ edges, Theorem 1 can be applied to it, resulting in:

Corollary 1.2. *Let $p \geq 5$ and let G be a (p,q)-graph. If $q \geq 2p$, then $L^2(G)$ is hyperenergetic.*

Continuing the same reasoning we obtain:

Corollary 1.3. *Let $p \geq 5$ and let G be a (p,q)-graph. If $q \geq 2p$, then all iterated line graphs $L^i(G)$, $i = 2, 3, \ldots$ are hyperenergetic.*

A REFINEMENT FOR BIPARTITE GRAPHS

If G is a bipartite graph, then Theorem 1 can slightly be improved.

Let G be a bipartite (p,q)-graph and let its vertex set be partitioned as $V = V_1 \cup V_2$, so that no two vertices from V_1 and no two vertices from V_2 are adjacent. Let W be the edge set of G. Define a p-dimensional vector $\mathbf{x} = (x_1, x_2, \ldots, x_p)$ as

$$x_i = \begin{cases} 1 & \text{if the } i\text{-th vertex belongs to } V_1 \\ -1 & \text{if the } i\text{-th vertex belongs to } V_2 \ . \end{cases}$$

Note that if $v_i \in V_1$ and $v_j \in V_2$, then $x_i + x_j = 0$. In particular, if $x_i x_j \in W$, then $x_i + x_j = 0$. Therefore,

$$\begin{aligned} \mathbf{x}^t\,(D(G) + A(G))\,\mathbf{x} &= \mathbf{x}^t R^t R\mathbf{x} = (R\mathbf{x})^t\,(R\mathbf{x}) \\ &= \sum_{v_i v_j \in W} (x_i + x_j)^2 = 0 \ . \end{aligned}$$

Hence, if G is bipartite, then $D(G) + A(G)$ is a singular matrix, that is, at least one eigenvalue of $D(G) + A(G)$ is equal to zero. Hence, $\mu_1 = 0$.

Bearing this fact in mind the inequality for the energy of $L(G)$, deduced in the previous section, can be somewhat improved:

$$\begin{aligned} E(L(G)) &= 2(q-p) + \sum_{i=1}^{p} |\mu_i - 2| = 2(q-p) + 2 + \sum_{i=2}^{p} |\mu_i - 2| \\ &\geq 2(q-p) + 2 + \sum_{i=2}^{p} (|\mu_i| - 2) = 2(q-p+1) + \sum_{i=2}^{p} (\mu_i - 2) \\ &= 2(q-p+1) + \sum_{i=2}^{p} \mu_i - 2(p-1) \end{aligned}$$

from which it follows

$$E(L(G)) \geq 4(q-p+1) \qquad \text{i. e.,} \qquad E(L(G)) \geq 2(q-1) + (2q-4p+6) \,. \tag{6}$$

From inequality (6) we see that if $2q - 4p + 6 > 0$, i. e., if $q \geq 2p - 2$, then $E(L(G)) > 2(q-1)$.

This time $q \leq p^2/4$ and if $q \geq 2p - 2$ then $p \geq 7$.

Theorem 2. *Let $p \geq 7$ and let G be a bipartite (p, q)-graph. If $q \geq 2(p-1)$, then $L(G)$ is hyperenergetic.*

DISCUSSION

The hyperenergetic graphs constructed as line graphs of some suitably chosen graphs usually possess fewer edges than the previously reported hyperenergetic graphs [9–13]. For instance, if G is a 4-regular $(p, 2p)$-graph, then $L(G)$ is a 6-regular $(2p, 6p)$-graph, that is, $L(G)$ is a hyperenergetic graph, and the number of its edges is only three times the number of its vertices.

Using a recently reported inequality [19], applicable to any (p, q)-graph,

$$E(G) \leq \frac{2q}{p} + \sqrt{(p-1)\left[2q - \left(\frac{2q}{p}\right)^2\right]}$$

we can easily show that if G is a $(p, 2p)$-graph, then $E(G) \leq 2p - 1$. We conjecture that there are no hyperenergetic $(p, 2p)$-graphs.

A interesting problem would be to characterize all graphs with hyperenergetic line graphs. This may not be easy because there exist (p, q)-graphs with $q < 2p$, such that their line graphs are hyperenergetic (cf. Fig. 2).

A related problem is to find the least integer $q(p)$, such that the line graph of any (p,q)-graph is hyperenergetic. For example, $q(5) = 9$ and $q(6) = 10$.

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