

More hyperenergetic molecular graphs

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If G is a molecular graph and $\lambda_1, \lambda_2, \dots, \lambda_n$ are its eigenvalues, then the energy of G is equal to $E(G) = |\lambda_1| + |\lambda_2| + \dots + |\lambda_n|$. This energy cannot exceed the value $n \sqrt{n-1} \approx n^{3/2}$. The graph G is said to be hyperenergetic if $E(G) > 2n - 2$. We describe the construction of hyperenergetic graphs G for which $E(G) \approx 1/2 n^{3/2}$.

Keywords: total π -electron energy, energy of graph, hyperenergetic graphs.

INTRODUCTION

Motivated by Monte Carlo studies¹ on the dependence of the average energy of a graph G on the parameters n (= the number of vertices of G) and m (= the number of edges of G), the concept of hyperenergetic graphs was put forward in a recent work.² The energy of a graph G with n vertices is defined as

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

where λ_i , $i = 1, 2, \dots, n$, are the eigenvalues of G ; for more details see Ref. 2 and the references quoted therein. A graph is said to be hyperenergetic if its energy, E , exceeds the energy of the complete graph with an equal number of vertices, *i.e.*, if $E > 2n - 2$.

It seems that no molecular graph representing a conjugated π -electron system is hyperenergetic. However, it was recently demonstrated^{2,3} that certain inorganic cluster graphs are hyperenergetic.

By generating, uniformly at random, (labeled) graphs with n vertices and m edges, it was possible to establish¹ the (n, m) -dependence of the average graph energy. Thus, if for a fixed value of n , $n \geq 10$, edges are added one-by-one at random, starting with n isolated vertices and ending with the complete graph, the average en-

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ergy increases, attains a maximum and then decreases. The maximal average energy was shown to increase as n .^{1,3} This analysis¹ indicated that amongst graphs with large numbers of edges, hyperenergetic graphs are frequently encountered. For an illustration see Fig. 1.

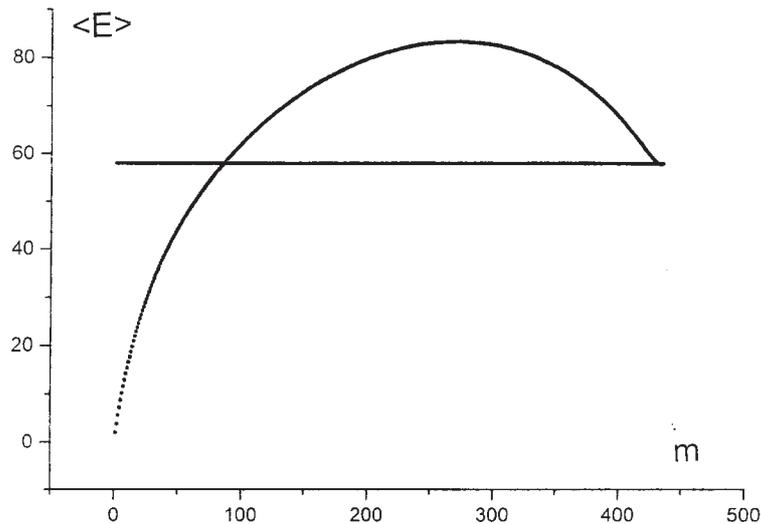


Fig. 1. The dependence of the average energy $\langle E \rangle$ of graphs with $n = 30$ vertices on $m =$ number of edges; energies above the horizontal line correspond to hyperenergetic graphs.

The next step in the study of this problem would be to find hyperenergetic graphs with very large energies, and if possible to find the n -vertex graph(s) with maximal energy. In connection with this it should be noted that from the McClelland inequality⁴

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

and the fact that the maximal number of edges in an n -vertex graph is $n(n-1)/2$ it immediately follows that

$$E \leq n\sqrt{n-1} \quad (2)$$

Hence, the maximal energy for an n -vertex graph cannot exceed $n\sqrt{n-1} \approx n^{3/2}$.

A CLASS OF HYPERENERGETIC GRAPHS WITH $E \approx 1/2 n^{3/2}$

A graph is said to be *regular* of degree r if each one of its vertices has degree (= number of adjacent vertices) equal to r . If a graph is regular it is said to be *strongly regular* if any two of its adjacent vertices are mutually adjacent to an equal number (say x) of other vertices, and if any two of its nonadjacent vertices are mutually adjacent to an equal number (say y) of other vertices.^{5,6}

Strongly regular graphs have only three distinct eigenvalues, and their spectra are fully determined by the parameters n, r, x, y .^{6,7} If $n = 4t + 1, r = 2t, x = t - 1$ and $y = t$, where t is a positive integer ($t = 1, 2, 3, \dots$), then the spectrum of the corresponding

strongly regular graph (when it exists) consists of the numbers:

$$2t; -\frac{1}{2}(1-\sqrt{4t+1}) \text{ (} 2t \text{ times)}; -\frac{1}{2}(1+\sqrt{4t+1}) \text{ (} 2t \text{ times)} \quad (3)$$

The above described graphs will be denoted by $Cf = Cf_n$; within mathematics these are called *conference graphs*. There are infinitely many graphs of this kind; for example, the highly symmetric *Paley graphs*,^{5,7,8} three examples of which are depicted in Fig. 2.

In view of relations (1) and (3), the energy of a conference graph with $4t + 1$

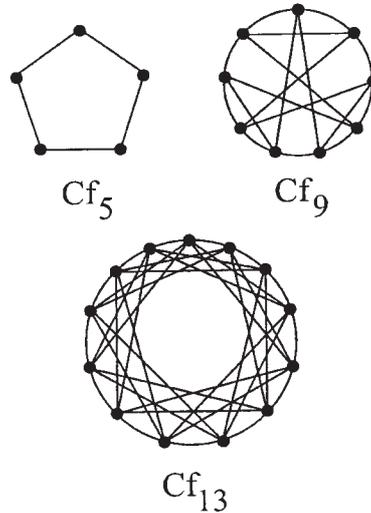


Fig. 2. Paley graphs with 5, 9 and 13 vertices; notice the 3-fold symmetry of Cf_9 and the 13-fold symmetry of Cf_{13} .

vertices is equal to

$$\begin{aligned} E(Cf) &= 2t + 2t \cdot \left| -\frac{1}{2}(1-\sqrt{4t+1}) \right| + 2t \cdot \left| -\frac{1}{2}(1+\sqrt{4t+1}) \right| \\ &= 2t + 2t \left[\frac{1}{2}(\sqrt{4t+1}-1) \right] + 2t \left[\frac{1}{2}(\sqrt{4t+1}+1) \right] \\ &= 2t + 2t\sqrt{4t+1} \end{aligned}$$

which results in

$$E(Cf_n) = \frac{1}{2}(n-1)(\sqrt{n}+1) \quad (4)$$

It is easy to verify that for $n \geq 3$ the right-hand side of Eq. (4) is greater than $1/2n\sqrt{n}$. Thus, Cf_n provides an example of a graph whose energy exceeds $1/2n^{3/2}$, that is, half the McClelland limit (2). At this moment these are the structurally fully characterized graphs with the highest known E -values.

DISCUSSION

The hyperenergetic graphs Cf_n described in the previous section exist only if $n = 4t + 1$, $t = 1, 2, 3, \dots$. Yet, the right-hand side of Eq. (4) can be calculated for any value of n , yielding an estimate of the energy of graphs whose structure does not differ much from those of conference graphs. These are given in Table I.

TABLE I. The energy $E(Cf_n)$, calculated according to Eq. (4), and the maximal energy $E_n(max)$ found by employing a random graph generator;¹ note that graphs of the type Cf_n exist only for $n = 5, 9, 13, 17, \dots$; the $E_n(max)$ -values for $n \leq 12$ are true maxima, whereas for $n \geq 13$ they are just the maximal observed energies in the computer experiments performed

n	$E(Cf_n)$	$E_n(max)$
5	6.4721	8.0000
6	8.6237	10.0000
7	10.9373	12.0000
8	13.3995	14.3253
9	16.0000	17.0600
10	18.7302	20.0000
11	21.5831	22.9175
12	24.5526	26.0000
13	27.6333	27.7244
14	30.8208	30.3281
15	34.1109	33.3798
16	37.5000	36.3271
17	40.9848	40.0686
18	44.5624	41.9915
19	48.2301	
20	51.9853	49.6559
21	55.8258	52.5173
22	59.7494	55.2864
23	63.7542	
24	67.8383	62.4321
25	72.0000	
26	76.2377	69.9061
27	80.5500	
28	84.9353	78.6999
29	89.3923	
30	93.9198	85.4227

In general, the energy of the graph Cf_n is not maximal. Within our Monte-Carlo type construction of (n, m) -graphs (the details of which are described elsewhere¹) graphs whose energies exceeded those of the conference graphs were encountered. The maximal observed graph energies (which need not be the true maxima) are also included in Table I.

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ИЗВОД

ЈОШ НЕКИ ХИПЕРЕНЕРГЕТСКИ МОЛЕКУЛСКИ ГРАФОВИ

ЧЕК Х. КОУЛЕН^а, ВИНЦЕНТ МОУЛТОН^б, ИВАН ГУТМАН^а и ДУШИЦА ВУДОВИЋ^а

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Нека је G молекулски граф и нека су $\lambda_1, \lambda_2, \dots, \lambda_n$ његове сопствене вредности. Енергија графа G је $E(G) = |\lambda_1| + |\lambda_2| + \dots + |\lambda_n|$. Ова енергија не може бити већа од $n\sqrt{n-1} \approx n^{3/2}$. За граф кажемо да је хиперенергетски ако је $E(G) > 2n - 2$. У овом раду описана је конструкција хиперенергетских графова за које је $E(G) \approx 1/2 n^{3/2}$.

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7. D. Cvetković, M. Doob, I. Gutman, A. Torgašev, *Recent Results in the Theory of Graph Spectra*, North-Holland, Amsterdam, 1988
8. A conference graph is of the *Paley type* if $n = 4t + 1$ is a prime power, if its vertex set equals the n -element finite field $GF(n)$, and if its edge set consists of those pairs of elements of $GF(n)$ whose difference is a square; for details see p. 10 of Ref. 5.