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Maximal Energy Graphs

Jack H. Koolen[1]

FSPM-Strukturbildungsprozesse, University of Bielefeld, D-33501 Bielefeld, Germany
E-mail: jkoolen@mathematik.uni-bielefeld.de

and

Vincent Moulton[2]

Department of Physics and Mathematics (FMI), Mid Sweden University, Sundsvall, S 851-70, Sweden
E-mail: vince@dirac.fmi.mh.se

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Given a graph G, its *energy* $E(G)$ is defined as the sum of the absolute values of the eigenvalues of G. The concept of the energy of a graph was introduced in the subject of chemistry by I. Gutman, due to its relevance to the total π-electron energy of certain molecules. In this paper, we show that if G is a graph on n vertices, then $E(G) \le (\frac{n}{2})(1+\sqrt{n})$ must hold, and we give an infinite family of graphs for which this bound is sharp.

Given a graph G, define the *energy of* G, denoted $E(G)$, by

$$E(G) := \sum_{\lambda \text{ an eigenvalue of } G} |\lambda|,$$

where the eigenvalues of G are simply those of the adjacency matrix of G. In chemistry, the energy of a given molecular graph is of interest since it can be related to the total π-electron energy of the molecule represented

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by that graph (see [7], for example). In [6, 11] *hyperenergetic* graphs, that is, graphs G on n vertices for which $E(G) > E(K_n) = 2n - 2$ holds, were considered. In particular, constructions were given that yield hyperenergetic graphs for each $n \geq 9$. However, even though energy theory for graphs is well developed—see [6] for an overview—relatively little is known concerning properties of graphs with maximal energy. Here we prove that if G is a graph on n vertices, then

$$E(G) \leq \frac{n}{2}(1 + \sqrt{n})$$

must hold, and that this bound is sharp if and only if G is strongly regular with parameters given by certain functions of n. This enables us to find an infinite family of maximal energy graphs.

We begin by recalling that a k-regular graph G on n vertices is called *strongly regular* with parameters (n, k, λ, μ) if the following conditions hold. Each pair of adjacent vertices has the same number $\lambda \geq 0$ of common neighbors, and each pair of non-adjacent vertices has the same number $\mu \geq 0$ of common neighbors. If $\mu = 0$, then G is a disjoint union of complete graphs, whereas, if $\mu \geq 1$ and G is non-complete, then the eigenvalues of G are k (the trivial eigenvalue) and the roots r, s of the quadratic equation

$$x^2 + (\mu - \lambda)x + (\mu - k) = 0. \tag{1}$$

The eigenvalue k has multiplicity one, whereas the multiplicities m_r of r and m_s of s can be calculated by solving the simultaneous equations

$$m_r + m_s = n - 1, \qquad k + m_r r + m_s s = 0$$

(for more details see [2, 3]).

THEOREM 1. *If $2m \geq n$ and G is a graph on n vertices with m edges, then the inequality*

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

holds. Moreover, equality holds in (2) if and only if G is either $\frac{n}{2}K_2$, K_n, or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{(2m - (\frac{2m}{n})^2)/(n-1)}$.

Proof. Suppose that $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ are the eigenvalues of G (which are real as the adjacency matrix of G is symmetric). Then, as is well known, we have

$$\eta_1 \geq \frac{2m}{n}$$

(see [4], for example). Moreover, since

$$\sum_{i=1}^{n} \eta_i^2 = 2m$$

must hold (for example, see [2]), we have

$$\sum_{i=2}^{n} \eta_i^2 = 2m - \eta_1^2.$$

Using this together with the Cauchy–Schwartz inequality, applied to the vectors $(|\eta_2|, \ldots, |\eta_n|)$ and $(1, 1, \ldots, 1)$ with $n-1$ entries, we obtain the inequality

$$\sum_{i=2}^{n} |\eta_i| \leq \sqrt{(n-1)(2m - \eta_1^2)}.$$

Thus, we must have

$$E(G) \leq \eta_1 + \sqrt{(n-1)(2m - \eta_1^2)}. \tag{3}$$

Now, since the function $F(x) := x + \sqrt{(n-1)(2m - x^2)}$ decreases on the interval $\sqrt{2m/n} < x \leq \sqrt{2m}$, in view of $2m \geq n$, we see that $\sqrt{2m/n} \leq 2m/n \leq \eta_1$ must hold, and hence $F(\eta_1) \leq F(2m/n)$ must hold as well. From this fact, and Inequality (3), it immediately follows that Inequality (2) holds.

We now consider what happens when equality holds in (2). As the eigenvalues for $\frac{n}{2}K_2$ are ± 1 (both with multiplicity $\frac{n}{2}$), and the eigenvalues of K_n are $n-1$ (multiplicity 1) and -1 (multiplicity $n-1$), it is easy to check that if G is one of the graphs given in the second part of the theorem, then equality must hold in (2).

Conversely, if equality holds in (2), then by the previous discussion on the function $F(x)$ we see that $\eta_1 = 2m/n$ must hold. It follows that G is regular with valence $2m/n$ [4]. Now, since equality must also hold in the Cauchy–Schwartz inequality given above, we have $|\eta_i| = \sqrt{(2m - (2m/n)^2)/(n-1)}$, for $2 \leq i \leq n$. Hence, we are reduced to three possibilities: either G has two eigenvalues with equal absolute values, in which case G must equal $(n/2)K_2$, or G has two eigenvalues with distinct absolute values, in which case G must equal K_n, or G has three eigenvalues with distinct absolute values equal to $2m/n$ or $\sqrt{(2m - (2m/n)^2)/(n-1)}$, in which case G must be a non-complete connected strongly regular graph (see [4]), as required. ∎

Remark 1. For a non-complete connected strongly regular graph G with parameters $\lambda = \mu$ it follows from the quadratic equation *(1)* and Theorem 1 that equality must hold for G in *(2)*. An infinite family of such strongly regular graphs is provided as follows: *Generalized quadrangles* with order $(t+2, t)$ exist for infinitely many $t \geq 1$ [1, 9]. Moreover, the point graph of a generalized quadrangle with order $(t+2, t)$ is strongly regular with parameters $((t+3)(t+1)^2, (t+1)(t+2), (t+1), (t+1))$; see [3, 1.15.1 Lemma].

In [8] McCelland proved that if G is a graph with n vertices and m edges, then the following bound must hold

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

If $2m \geq n$, then using the Cauchy–Schwartz inequality in a similar fashion to the way in which it was used in the proof of Theorem 1, together with the equality

$$\sum_{i=1}^{n} \eta_i^2 = 2m,$$

the McCelland inequality is easily recovered, and it is immediately seen that equality holds if and only if $G = (n/2)K_2$. Moreover, since $F(\sqrt{2m/n}) = \sqrt{2mn}$ holds for the function F defined in the proof of Theorem 1, and, as stated in the proof, since F decreases on the interval $\sqrt{2m/n} < x \leq \sqrt{2m}$, it follows from Inequality (3) that

$$\frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} \leq \sqrt{2mn} \tag{4}$$

must hold, so that Inequality (2) is an improvement on the McCelland bound. Also, considering the function F once more, we see that equality holds in (4) if and only if $2m = n$ and $G = (n/2)K_2$.

In Theorem 1 we considered only the case $2m \geq n$; we now look at what happens when this inequality is reversed:

THEOREM 2. *If $2m \leq n$ and G is a graph on n vertices with m edges, then the inequality*

$$E(G) \leq 2m \tag{5}$$

holds. Moreover, equality holds in (5) if and only if G is disjoint union of edges and isolated vertices.

Proof. Since $2m \le n$, it follows that G must have at least $n-2m$ isolated vertices. Consider the graph G' that is obtained from G by removing $n-2m$ isolated vertices. Then G' has $2m$ vertices and m edges. Thus we may apply Theorem 1 to immediately see that $E(G') \le 2m$ must hold, with equality holding if and only if G' is the disjoint union of edges. The proof of the theorem now immediately follows. ∎

Note that since a graph G on n vertices has at most $(n(n-1))/2$ edges it follows from McCelland's bound that the inequality

$$E(G) \le n\sqrt{n-1}$$

must hold. We now see that Inequality (2) allows us to improve on this bound, and in the process yield the main result of this paper:

THEOREM 3. *Let G be a graph on n vertices. Then*

$$E(G) \le \frac{n}{2}(1+\sqrt{n}) \tag{6}$$

holds, with equality holding if and only if G is a strongly regular graph with parameters $(n, (n+\sqrt{n})/2, (n+2\sqrt{n})/4, (n+2\sqrt{n})/4)$.

Proof. Suppose that G is a graph with n vertices and m edges.

If $2m \ge n$, then using routine calculus, it is seen that the left hand side of Inequality (2)—considered as a function of m—is maximized when

$$m = \frac{n^2 + n\sqrt{n}}{4}$$

holds. Inequality (6) now follows by substituting this value of m into (2). Moreover, it follows by Theorem 1 and (1) that equality holds in (6) if and only if G is a strongly regular graph with parameters $(n, (n+\sqrt{n})/2, (n+2\sqrt{n})/4, (n+2\sqrt{n})/4)$.

If $2m \le n$, then by Theorem 3, $E(G) \le n$. The proof of the theorem now follows immediately. ∎

Remark 2. The graphs for which equality is attained in Theorem 3 are strongly regular with parameter $\mu = r(r+1)$, and are therefore strongly regular graphs of negative Latin square type.

Using Theorem 3, we now provide an infinite family of maximal energy graphs that arises from the theory of *semipartial geometries* [5]. For each $m \ge 1$, there exists a semipartial geometry with parameters

$$\left(2^{m+1}-1, 2^{m+2}, 2^m, 2^{m+1}(2^{m+1}-1)\right)$$

(see [5; p. 456; 10]). The point graph of this geometry is a strongly regular graph with parameters $(4\tau^2, (\tau-1)(2\tau+1), (\tau-2)(\tau+1), \tau(\tau-1))$

where $\tau := 2^{m+1}$; see [5, p. 449]. The complement of this graph is also strongly regular with parameters $(4\tau^2, \tau(2\tau+1), \tau(\tau+1), \tau(\tau+1))$. Thus by Theorem 3, these graphs form an infinite sequence of graphs for which Inequality (6) is sharp.

In conclusion, note that the bounds given in this paper can be clearly considered for special classes of graphs such as bipartite graphs; more details on this will appear elsewhere. Also, for given $\epsilon > 0$ we suspect that for almost all $n \geq 1$ there exists a graph G on n vertices for which $E(G) \geq (1-\epsilon)(n/2)(1+\sqrt{n})$.

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REFERENCES

1. R. Ahrens and G. Szekeres, On a combinatorial generalization of 27 lines associated with a cubic surface, *J. Austral. Math. Soc.* **10** (1969), 485–492.
2. N. Biggs, "Algebraic Graph Theory," Cambridge Univ. Press, Cambridge, UK, 1993.
3. A. Brouwer, A. Cohen, and A. Neumaier, "Distance Regular Graphs," Springer-Verlag, New York/Berlin, 1989.
4. D. Cvetkovic, M. Doob, and H. Sachs, "Spectra of Graphs—Theory and Application," Academic Press, San Diego, 1995.
5. F. De Clerck and H.Van Maldeghem, Some classes of rank 2 geometries, *in* "Handbook of Incidence Geometry," Elsevier, Amsterdam/New York, 1995.
6. I. Gutman, Hyperenergetic molecular graphs, *J. Serb. Chem. Soc.* **64** (1999), 199–205.
7. I. Gutman, The energy of a graph: Old and new results, preprint.
8. B. McCelland, Properties of the latent roots of a matrix: The estimation of π-electron energies, *J. Chem. Phys.* **54** (1971), 640–643.
9. S. Payne, Nonisomorphic generalized quadrangles, *J. Algebra* **18** (1971), 201–212.
10. J. Thas, Semi-partial geometries and spreads of classical polar spaces, *J. Combin. Theory Ser. A* **35** (1983), 58–66.
11. H. Walikar, H. Ramane, and P. Hampiholi, On the energy of a graph, *in* "Graph Connections," Allied Publishers, New Delhi, 1999.