Graphs with extremal energy should have a small number of distinct eigenvalues

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Abstract

The sum of the absolute values of the eigenvalues of a graph is called the energy of the graph. We study the problem of finding graphs with extremal energy within specified classes of graphs. We develop tools for treating such problems and obtain some partial results. Using calculus, we show that an extremal graph "should" have a small number of distinct eigenvalues. However, we also present data that shows in many cases that extremal graphs can have a large number of distinct eigenvalues.[1]

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1 Introduction

Let G be a simple undirected graph on n vertices with $m > 0$ edges. Let $x_1, x_2, \ldots, x_n$ be the eigenvalues of G. Let $I = \{1, 2, \ldots, n\}$.

The following relations are well-known:

$$\sum_{i \in I} x_i = 0, \tag{1}$$

$$\sum_{i \in I} x_i^2 = 2m. \tag{2}$$

[1]The idea for this note arose during the workshop "Spectra of families of matrices described by graphs, digraphs, and sign patterns" which was held at American Institute of Mathematics in Palo Alto, California, U.S.A. on October 23–27, 2006.

The energy $E(G)$ of G is defined by

$$E(G) = \sum_{i \in I} |x_i|.$$

The energy of a graph was defined by I. Gutman [4] and has attracted much attention from researchers in the last few years.

Given a set $\mathcal{G}$ of graphs, one can ask which graphs in $\mathcal{G}$ have extremal (minimal or maximal) energy. In this paper, we shall develop a procedure for treating the problem of finding an extremal graph when all graphs in $\mathcal{G}$ have a fixed number of vertices and edges and a given family of eigenvalues. Because our procedure allows us to specify eigenvalues that graphs in $\mathcal{G}$ must have, we can make sure that $\mathcal{G}$ includes all graphs having certain properties (bipartite, regular, etc.). Because our procedure relies on methods of continuous calculus, it will not always produce a graph with extremal energy. However, even when we do not obtain a graph with extremal energy, our procedure still gives a heuristic to guide a search for such a graph.

We will concentrate our efforts in this paper on finding a graph in $\mathcal{G}$ that has maximal energy. Our tools can also be applied to the problem of finding graphs with a minimal energy. However, this problem appears to be easier and there are several recent results in this direction (see, for example, [11], [6]), so we shall mention it only in passing.

It is known that for $n \leq 7$, the graphs with maximal energy are the complete graphs K_n, $n = 1, 2, \ldots, 7$. Maximal values of energy for graphs with n vertices have been determined heuristically by the system AutoGraphiX [1] for $n \leq 12$. In [1], the corresponding maximal energy graph is given only for $n = 10$. The graph with maximal energy among 10-vertex graphs is the complement of the Petersen graph, i.e., the line graph $L(K_5)$ of the complete graph K_5. This graph is strongly regular and has three distinct eigenvalues. Maximal energy graphs have been determined in [7] for an infinite sequence of values of n (n is a power of 2) and in these cases the graphs are also strongly regular. The smallest such graph, the Clebsch graph, has 16 vertices and the spectrum $10, 2^5, -2^{10}$ (superscripts denote multiplicities of eigenvalues). The Clebsch graph appears as graph No. 187 in Table A3 in [3].

The connection between maximal energy graphs and strong regularity is explored further in [7]. It is proved in [7] that for a graph G on n vertices the following inequality holds:

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

with equality if and only if G is a strongly regular graph with parameters $(n, (n+\sqrt{n})/2, (n+\sqrt{n})/4, (n+\sqrt{n})/4)$. Such strongly regular graphs exist for $n = 4\tau^2$ for $\tau = 2^m$, $m = 1, 2, \ldots$. From the theory of strongly regular graphs, one can deduce that a graph with such parameters has distinct eigenvalues $\tau(2\tau+1), \pm\tau$. The conjecture that, for any $\epsilon > 0$, for almost all n, there exists a graph G on n vertices such that

$$E(G) \geq (1-\epsilon)\frac{n}{2}(1+\sqrt{n})$$

has been confirmed in a slightly improved form in [10]. These results give a basis to think that, in general, graphs with extremal energy have a small number of distinct eigenvalues. Though our results support this heuristic, we also note examples with significant deviations from these expectations. These unexpected examples seem to make the maximal energy problem very difficult.

The rest of the paper is organized as follows. In Section 2, we present some known results on graph spectra which will be used later. In Section 3, we prove a simple but useful theorem which gives a basis for thinking that extremal graphs should have a small number of distinct eigenvalues. Section 4 contains examples using our theorem. In Section 5, we present some computational and theoretical data which show the existence of maximal energy graphs with a large number of distinct eigenvalues. A heuristic procedure for finding maximal energy graphs is formulated in Section 6. Finally, we summarize our main points concerning maximal energy graphs in Section 7.

2 Preliminaries

We shall quote some simple and well-known facts from the theory of graph spectra which will be used in the rest of the paper.

Proposition 1. (see [2], p. 85) *For any graph with eigenvalues $x_1, x_2, \ldots, x_n$ and t triangles we have $\sum_{i\in I} x_i^3 = 6t$.*

In particular, this means that the third spectral moment $\sum_{i\in I} x_i^3$ is always an integer that is divisible by 6.

Proposition 2. (see [2], p. 87) *A graph is bipartite if and only if its spectrum is symmetric with respect to 0.*

In bipartite graphs, if x is an eigenvalue of multiplicity k, then $-x$ is also an eigenvalue of multiplicity k.

Proposition 3. (see [2], p. 94) *A graph with n vertices, m edges, and largest eigenvalue x_1 is regular if and only if $x_1 = \frac{2m}{n}$.*

Proposition 4. (see [2], p. 56) *If G is a regular graph with eigenvalues $x_1, x_2, \ldots, x_n$ (with $x_1 \geq x_i$ for $i = 2, \ldots, n$), then the eigenvalues of the complement of G are $n - x_1 - 1$ and $-x_i - 1$ for $i = 2, \ldots, n$.*

Proposition 5. (see [2], p. 53) *The eigenvalues of a cycle C_n of length n are $2\cos\left(\frac{2\pi}{n}j\right)$, where $j = 1, 2, \ldots, n$.*

In particular, we obtain the spectrum for a triangle $(2, -1^2)$, a quadrangle $(2, 0^2, -2)$, and a pentagon $(2, 0.618^2, -1.618^2$, i.e., $2, (1/\varphi)^2, -\varphi^2$, where $\varphi = (1+\sqrt{5})/2 \approx 1.618$, the golden ratio).

3 Main theorem and tools

To motivate our main theorem, we shall use traditional calculus to try to find extremal values of the energy of graphs. Of course, using techniques from continuous mathematics in problems of discrete mathematics requires careful handling and we shall see the limitations of such an approach. However, some results can be achieved. The use of calculus in handling extremal problems with graph eigenvalues was suggested in [2, Section 7.7].

Define

$$I = I_+ \cup I_-, \text{ where}$$

$$I_+ = \{i | i \in I, x_i \geq 0\} \quad \text{and} \quad I_- = \{i | i \in I, x_i < 0\}.$$

Then the energy can be represented in the following form:

$$E = \sum_{i \in I_+} x_i - \sum_{i \in I_-} x_i.$$

If the graph is not trivial, then I_+ and I_- are both non-empty by (1).

Consider an auxiliary function involving the constraints (1) and (2):

$$F = \sum_{i \in I_+} x_i - \sum_{i \in I_-} x_i + \alpha \sum_{i \in I} x_i + \beta \left(\sum_{i \in I} x_i^2 - 2m \right),$$

where α, β are Lagrange multipliers. Extremal values of the function E satisfying the constraints (1) and (2) can be found by equating the partial derivatives of function F with 0, i.e.

$$\frac{\partial F}{\partial x_j} = \pm 1 + \alpha + 2\beta x_j = 0, \quad j \in I.$$

The first term in the sum is equal to $+1$ if $j \in I_+$ and is equal to -1 if $j \in I_-$. Hence we obtain

$$x_j = \frac{-\alpha \mp 1}{2\beta}, \quad j \in I.$$

This means that a graph with extremal energy should have only two distinct eigenvalues.

These derivations were used in [5] to derive the McClelland upper bound for the energy in a new way.

However, the only graphs that have only two distinct eigenvalues are unions of complete graphs of a fixed order. We must assume that at least three distinct eigenvalues exist in non-trivial cases.

We shall treat our problem in the following way. Assume that we somehow know that an extremal graph we are looking for has some fixed and given eigenvalues $\mathcal{K}$, consisting of x_i, $i \in K$. Let $\mathcal{H}$ be the set of graphs having a fixed number of vertices and edges and the given family of eigenvalues $\mathcal{K}$. Let $J = I \setminus K$, so that the eigenvalues x_i, $i \in J$, are considered unknown. We seek to determine these unknown eigenvalues in such a way that the energy becomes extremal in $\mathcal{H}$. Index sets J and K are further partitioned, as I was partitioned, into subsets corresponding to non-negative and negative eigenvalues:

$$J = J_+ \cup J_- \quad \text{and} \quad K = K_+ \cup K_-.$$

Now we have

$$E = \sum_{i \in J_+} x_i - \sum_{i \in J_-} x_i + \sum_{i \in K_+} x_i - \sum_{i \in K_-} x_i,$$

and from (1) and (2),

$$\sum_{i \in J} x_i + \sum_{i \in K} x_i = 0 \quad \text{and} \quad \sum_{i \in J} x_i^2 + \sum_{i \in K} x_i^2 = 2m.$$

Let

$$C_+ = \sum_{i \in K_+} x_i, \; C_- = \sum_{i \in K_-} x_i, \; C = \sum_{i \in K} x_i, \text{ and } D = \sum_{i \in K} x_i^2. \tag{3}$$

We can write

$$F = \sum_{i \in J_+} x_i - \sum_{i \in J_-} x_i + C_+ - C_- + \alpha \left(\sum_{i \in J} x_i + C \right) + \beta \left(\sum_{i \in J} x_i^2 + D - 2m \right).$$

Using partial derivatives for any $j \in J$, we get

$$\frac{\partial F}{\partial x_j} = \pm 1 + \alpha + 2\beta x_j = 0 \implies x_j = \frac{-\alpha \mp 1}{2\beta}.$$

Assuming that both sets J_+ and J_- are non-empty, this means that unknown eigenvalues should have only two values in a graph with extremal energy. (Sometimes one of the sets J_+ or J_- is empty in which case our approach does not give any solution.) Denote the two values obtained by x, y and the corresponding multiplicities by p, q.

This sets up $|J| - 1$ Lagrange multiplier problems (one for each situation $|J_+| = i$ and $|J_-| = |J| - i$ for $i = 1, 2, \ldots, |J| - 1$). For a given distribution of unknown positive and negative eigenvalues, the solution of the corresponding Lagrange multiplier problem will give us an upper bound on the maximal energy of graphs in $\mathcal{H}$ with a corresponding distribution of unknown eigenvalues. If we take the maximal value E over all such solutions, and that energy value is realized by a graph, then we know we have a maximal energy graph in $\mathcal{H}$.

Extend the known part of the spectrum $\mathcal{K}$ by the values corresponding to E of x, y with multiplicities p, q. Denote by L the described procedure of completing the partial spectrum using the Lagrange multipliers and let $\mathcal{K}_L$ be the resulting complete spectrum.

Now we can formulate a slightly more general statement.

Theorem 1. *Let n, m be positive integers and let $\mathcal{K}$ be a family of reals. Let $\mathcal{G}$ be the class of graphs having n vertices and m edges. Suppose that $G \in \mathcal{G}$ is a graph with maximal energy in $\mathcal{G}$ and has all members of $\mathcal{K}$ as eigenvalues. Let $\mathcal{K}_L$ be the spectrum obtained from $\mathcal{K}$ by procedure L. If a graph H has the spectrum $\mathcal{K}_L$, then H also has maximal energy in $\mathcal{G}$ and has the same energy as G.*

Proof. Suppose that $G \in \mathcal{G}$ is a maximal energy graph in $\mathcal{G}$ with energy E. Let $\mathcal{H}$ be the class of graphs from $\mathcal{G}$ which have all members of $\mathcal{K}$ as eigenvalues. By the construction of $\mathcal{K}_L$, the graph H belongs to $\mathcal{H}$ and has a maximal energy in $\mathcal{H}$. Since $G \in \mathcal{H}$, H must have energy at least E. However, since G is also a maximal graph in $\mathcal{G}$, the energy of H must be exactly equal to E, so H also is a maximal graph in $\mathcal{G}$. □

An analagous procedure and theorem can be stated for minimal energy graphs.

This theorem can be interpreted as "graphs with extremal energy *should* have a small number of distinct eigenvalues," as pointed out in the title of this paper. Namely, the eigenvalues which are not fixed by the set $\mathcal{K}$ would have, in a truly optimal graph, only two values, if such a graph happened to exist.

4 Examples

In this section we shall give several examples of using Theorem 1 to guide searches for maximal energy graphs. Note that these examples may not represent complete proofs that the graphs involved have extremal energy. However, they do illustrate how to use the ideas behind Theorem 1.

As a computational alternative, instead of explictly using procedure L and the involved Lagrange equations, we will compute all possible ways of adding two eigenvalues to the family $\mathcal{K}$ while respecting the constraints (1) and (2). The solutions of the Lagrange equations in procedure L will be among these results, so maximizing the energy over these results will yield the maximum we would get from procedure L.

To this end, we introduce some technical notation. The set J contains $|J| = n - |K|$ elements. Suppose that an extremal solution contains eigenvalues x, y with multiplicities p, q respectively. The following system of equations must be satisfied, where p, q, and $|J|$ are positive integers and x, y, C, and D are real numbers:

$$\{p + q = |J|,\, px + qy = -C,\, px^2 + qy^2 = 2m - D\}. \tag{4}$$

In this notation, the energy is $E = p|x| + q|y| + C_+ - C_-$.

Our examples are computed using a small Mathematica program (see Appendix A) or a small SAGE [9] program (see Appendix B). Given the number of vertices, the number of edges, and a list of known eigenvalues that define $\mathcal{G}$, the program prints all 4-tuples (p, q, x, y) satisfying the system of equations (4). For each solution, the program also prints the corresponding energy E and $\frac{1}{6}\sum_{i\in I} x_i^3$. This last quantity is the third spectral moment divided by 6 and should be an integer if the solution corresponds to the eigenvalues of an actual graph (see Proposition 1). To solve the system of equations, we vary p between 1 and $|J| - 1$ and for each such p corresponding solutions are obtained (0, 1 or 2 solutions, having in mind that the third equation in (4) is quadratic). However, because of the symmetry of the system of equations, it is sufficient to consider solutions for $p = 1, 2, \ldots, \lfloor |J|/2 \rfloor$.

A. Let us examine the class of regular graphs of degree 10 having 16 vertices. By Proposition 3, the class $\mathcal{G}$ defined by $n = 16$, $m = 80$, and $\mathcal{K} = \{10\}$

coincides with this class. This implies that $|K| = 1$, $|J| = 15$, $C = 10$, and $D = 100$. Our program gives the following results.

p	q	x	y	E	$\frac{1}{6}\left(\sum_{i=1}^{n} x_i^3\right)$
1	14	−7.7220	−0.1627	20.0000	89.9136
1	14	6.3887	−1.1706	32.7773	206.3830
2	13	−5.4741	0.0729	21.8963	111.9900
2	13	4.1407	−1.4063	36.5629	184.3060
3	12	−4.4379	0.2761	26.6274	123.0070
3	12	3.1046	−1.6095	38.6274	173.2900
4	11	−3.7936	0.4704	30.3489	130.4600
4	11	2.4603	−1.8037	39.6822	165.8360
5	10	−3.3333	0.6667	33.3333	136.2960
5	10	2.0000	−2.0000	40.0000	160.0000
6	9	−2.9761	0.8729	35.7128	141.3050
6	9	1.6427	−2.2063	39.7128	154.9910
7	8	−2.6825	1.0972	37.5547	145.9080
7	8	1.3491	−2.4305	38.8880	150.3880

The value $p = 5$ corresponds to the maximal energy $E = 40$ and we get the Clebsch graph with the spectrum $10, 2^5, -2^{10}$. There are no other graphs with this spectrum [3].

B. Consider now graphs on $n = 10$ vertices.

1. $m = 30$ edges.

A maximal energy graph in $\mathcal{G}$ cannot be complete. Therefore it must have at least three distinct eigenvalues. Restrict our search further to connected graphs with largest eigenvalue 6 (which is simple). Then $\mathcal{K} = \{6\}$. (The complement of the Petersen graph is in $\mathcal{G}$.) Now we have $|K| = 1$, $|J| = 9$, $C = 6$, and $D = 36$. Our program gives the following solutions.

p	q	x	y	E	$\frac{1}{6}\left(\sum_{i=1}^{n} x_i^3\right)$
1	8	−4.8830	−0.1396	12.0000	16.5911
1	8	3.5497	−1.1937	19.0994	41.1866
2	7	−3.4555	0.1302	13.8221	22.2487
2	7	2.1222	−1.4635	20.4888	35.5290
3	6	−2.7749	0.3874	16.6491	25.3752
3	6	1.4415	−1.7208	20.6491	32.4025
4	5	−2.3333	0.6667	18.6667	27.7778
4	5	1.0000	−2.0000	20.0000	30.0000

High values of energy are obtained for $p = 3$ and $p = 2$, but the corresponding graphs do not exist since the third spectral moment is not divisible by 6 (cf. Proposition 1). For $p = 4$, we find that $L(K_5)$, the line graph of the complete graph K_5, has distinct eigenvalues 6, 1, -2 with multiplicities 1, 4, 5 respectively. The graph $L(K_5)$ is known to have maximal energy among all 10 vertex graphs [1].

One should be aware that our calculations do not prove that $L(K_5)$ has maximal energy (this fact we know from [1]). If a graph existed that had spectrum 6, 1.4415^3, -1.7208^6, then Theorem 1 would establish it as a maximal energy graph over $\mathcal{G}$. However, we do not know if there is a graph with, say, eight distinct eigenvalues (all but one close to 1.4415 or -1.7208) which could have energy very close 20.6491. It seems that one has to introduce a kind of distance between spectra (families of reals) to handle such effects, but we shall not do that in this paper.

2. $m = 9$ edges.

Restrict our search to graphs having a simple eigenvalue $\mathcal{K} = \{3\}$. Thus $|K| = 1$, $|J| = 9$, $C = 3$, and $D = 9$. We then get the following solutions.

p	q	x	y	E	$\frac{1}{6}\left(\sum_{i=1}^{n} x_i^3\right)$
1	8	-3.0000	0.0000	6.0000	0.0000
1	8	2.3333	-0.6667	10.6667	6.2222
2	7	-2.0972	0.1706	8.3887	1.4313
2	7	1.4305	-0.8373	11.7220	4.7910
3	6	-1.6667	0.3333	10.0000	2.2222
3	6	1.0000	-1.0000	12.0000	4.0000
4	5	-1.3874	0.5099	11.0994	2.8300
4	5	0.7208	-1.1766	11.7661	3.3922

For $p = 1$ we get the star $K_{1,9}$ (in accordance with the known fact that stars are minimal energy graphs among the trees with a fixed number of vertices) and for $p = 3$, we get that the graph $K_4 \cup 3K_2$ has maximal energy (among graphs considered).

C. The procedure developed is very flexible in the sense that some structural restrictions on graphs (e.g., regularity, bipartiteness, connectedness, etc.) can easily be introduced. Consider graphs on $n = 14$ vertices with $m = 21$ edges. If we apply Theorem 1 with $\mathcal{K} = \emptyset$ (general graphs), and $\mathcal{K} = \{3\}$ (cubic graphs, cf. Proposition 3), we do not get any graphs. However, if we assume $\mathcal{K} = \{3, -3\}$ (cubic bipartite graphs, cf. Proposition 2), we obtain

Vertices	Graph6	Edges	Energy	Distinct Eigenvalues	Spectrum
7	F`~~w	17	12	4	$5, 1, -1^4, -2$
8	G`lv~{	21	14.325	7	5.427, 1.118, 0.618, -1^2, -1.618, -1.679, -1.865
9	HEutZhj	21	17.060	6	4.702, 1.414^2, 1, -1.414^2, -1.702, -2^2
10	I~qkzXZLw	30	20	3	$6, 1^4, -2^5$
11	JJ^em]uj[v_	36	22.918	5	6.585, 1.874, 1^3, -1.459, -2^5
12	K~z\c\qRXVa~	42	26	5	7, 2^2, 1^2, -1, -2^6

Table 1: Maximal energy graphs

the Heawood graph with eigenvalues $3, \sqrt{2}^6, -\sqrt{2}^6, -3$, which really is an extremal graph.

5 Some data on maximal energy graphs

The presented material might suggest that graphs with extremal energy always have a small number of distinct eigenvalues. We now present some computational and theoretical facts showing that this is not always the case.

We present in Table 1 results of computations concerning extremal energy graphs up to $n = 12$ vertices, performed when the paper [1] was being prepared, but which have not been published. Each graph is identified with a graph6 code, which is a compact representation of the adjacency matrix. The specification of the graph6 code is distributed with Brendan McKay's Nauty program [8] and can also be found on the Nauty website. We have independently verified these results with our own computer programs by an exhaustive search. For $n = 11, 12$ we reduced the search to specific numbers of edges ($m = 35, 36, 37$ for $n = 11$ and $m = 41, 42, 43$ for $n = 12$—about 4.6 billion graphs in the latter case).

We note a few items of interest from Table 1. For $n = 7$ there exists a graph with the spectrum $5, 1, -1^4, -2$ which has the same (maximal) energy ($E = 12$) as the complete graph K_7. For $n = 12$ the extremal graph is regular of degree 7. This graph is known as an exceptional graph for the least eigenvalue -2 and can be found as graph No. 186 in Table A3 of [3]. In these examples, the eigenvalue -2 almost always appears with high multiplicity. The number -2 is the least eigenvalue in almost all line graphs. For the role of the number -2 in the theory of graph spectra, see [3].

This data partially confirms the tendency of eigenvalues of high multiplicity (i.e., small number of distinct eigenvalues) in maximal energy graphs. However, some cases in which there are a large number of distinct eigenvalues also occur. Another example of graphs with maximal energy and a high number of distinct eigenvalues is known from theoretical considerations. Among trees with a given number of vertices, the path has maximal energy (cf., e.g., [2], p. 238).

Examples with a high number of distinct eigenvalues show that, in these cases, several sets of eigenvalues produced by procedure L by specifying families of eigenvalues $\mathcal{K}$ do not actually correspond to graphs. This can be seen in the case of a path in the following way. Let $\pi_1, \pi_2, \ldots, \pi_n$ be (distinct) eigenvalues of a path P_n on n vertices. Let $\mathcal{K}_i = \{\pi_1, \pi_2, \ldots, \pi_i\}, i = 1, 2, \ldots, n-2$. By applying procedure L in turn with these sets we come to P_n only after $n-2$ iterations.

6 A heuristic procedure

Having in view all that has been said, one can outline the following heuristic procedure for finding extremal graphs by repeated applications of procedure L.

Procedure. *Let n, m be positive integers and let $\mathcal{K}$ be the family of reals. Let $\mathcal{K}_L$ be the eigenvalues derived from procedure L. Try to construct a graph having eigenvalues $\mathcal{K}_L$. If such a graph does not exist, repeatedly add eigenvalues to $\mathcal{K}$ and try to construct a graph with eigenvalues $\mathcal{K}_L$.*

Of course, depending on the concrete problem, the eigenvalues to add to $\mathcal{K}$ should be determined with other facts and tools not contained in Theorem 1.

We shall give an example of using this procedure to determine a regular graph of degree 15 on 18 vertices with maximal energy. Since the complement of such a graph is regular of degree 2, we know that the complement of such a graph is composed of disjoint unions of cycles. Hence we could apply our Mathematica program a few times while trying, for example, the presence of eigenvalues $-\varphi \approx -1.618, 1/\varphi \approx 0.618$, which come from a pentagon in the complement, and/or $1, -1$, which come from a quadrangle in the complement (cf. Propositions 4 and 5). However, we will try to use procedure L to guide our guesses.

Using our Mathematica program with $n = 18$, $m = 15n/2 = 135$ and $\mathcal{K} = \{15\}$, we have the following solutions:

p	q	x	y	E	$\frac{1}{6}\left(\sum_{i=1}^{n} x_i^3\right)$
1	16	−6.3501	−0.5406	30.0000	519.4020
1	16	4.5854	−1.2241	39.1708	573.6770
2	15	−4.6259	−0.3832	30.0000	529.3640
2	15	2.8612	−1.3815	41.4446	563.7160
3	14	−3.8353	−0.2496	30.0000	534.2570
3	14	2.0706	−1.5151	42.4234	558.8230
4	13	−3.3466	−0.1241	30.0000	537.5080
4	13	1.5819	−1.6406	42.6554	555.5720
5	12	−3.0000	0.0000	30.0000	540.0000
5	12	1.2353	−1.7647	42.3529	553.0800
6	11	−2.7332	0.1272	32.7983	542.0860
6	11	0.9685	−1.8919	41.6218	550.9940
7	10	−2.5162	0.2613	35.2261	543.9450
7	10	0.7514	−2.0260	40.5203	549.1350
8	9	−2.3322	0.4064	37.3153	545.6870
8	9	0.5675	−2.1711	39.0800	547.3930

As we can see, the only solution that passes the 3rd moment test is $p = 5$, $q = 12$, $x = -3$, $y = 0$, and $E = 30$. Interestingly, this is the lowest energy solution found. We have obtained the eigenvalues of the graph $\overline{6C_3}$ with the spectrum $15, 0^{12}, -3^5$. It has three distinct eigenvalues and belongs to the set of trivial strongly regular graphs.

By Propositions 3 and 4, a 15-regular 18-vertex graph has eigenvalue -3 with multiplicity k if and only if the complement of the graph has $k+1$ components (which are all cycles). Let us assume for the moment that our extremal graph has at least 4 components in its complement. Therefore we take $\mathcal{K} = \{15, -3, -3, -3\}$. We have the following computer output (in the tables below, the lines in which the third spectral moment is divisible by 6 will be denoted by $+$ and the others will be denoted by $-$).

p	q	x	y	E	3rd moment test
1	13	−4.2136	−0.1374	30.0000	−
1	13	3.3565	−0.7197	36.7129	−
2	12	−3.0000	0.0000	30.0000	+
2	12	2.1429	−0.8571	38.5714	−
3	11	−2.4387	0.1197	32.6325	−
3	11	1.5816	−0.9768	39.4896	−
4	10	−2.0884	0.2354	34.7074	−
4	10	1.2313	−1.0925	39.8502	−
5	9	−1.8370	0.3539	36.3700	−
5	9	0.9799	−1.2110	39.7986	−
6	8	−1.6408	0.4806	37.6891	−
6	8	0.7836	−1.3377	39.4033	−
7	7	−1.4784	0.6212	38.6969	−
7	7	0.6212	−1.4784	38.6969	−

Note that third line passes the 3rd moment test and yields again $\overline{6C_3}$.

The second line for $p = 6$ shows that we can get high energy solutions if we have a group of six eigenvalues around 0.7836 and a group of eight eigenvalues around −1.3377. This can be roughly achieved if we assume the existence of two pentagons in the complement. By Proposition 4, each pentagon in the complement will introduce two eigenvalues of $\varphi - 1 \approx 0.618$ and two eigenvalues of $-1/\varphi - 1 = -\varphi \approx -1.618$. Therefore we take

$$\mathcal{K} = \{15, -3, -3, -3, \varphi - 1, \varphi - 1, \varphi - 1, \varphi - 1, -\varphi, -\varphi, -\varphi, -\varphi\}$$

which yields

p	q	x	y	E	3rd moment test
1	5	−2.4415	0.0883	35.8273	−
1	5	1.7749	−0.7550	38.4940	−
2	4	−1.6667	0.3333	37.6109	−
2	4	1.0000	−1.0000	38.9443	+
3	3	−1.2761	0.6095	38.6011	−
3	3	0.6095	−1.2761	38.6011	−

Note that the fourth line:

$$2 \quad 4 \quad 1.0000 \quad -1.0000 \quad 38.9443 \quad +$$

passes the 3rd moment test. This spectrum is realized by the complement of $2C_4 \cup 2C_5$. Through an exhaustive search, we have verified that this graph has maximal energy among all regular graphs of degree 15 on 18 vertices. This extremal graph, $\overline{2C_4 \cup 2C_5}$, has 6 distinct eigenvalues and spectrum $15, 1^2, (\varphi-1)^4, -1^4, -\varphi^4, -3^3$ (cf. Propositions 4 and 5).

We could have approached this another way. If we assume the presence of two quadrangles by letting

$$\mathcal{K} = \{15, -3, -3, -3, -1, -1, -1, -1, 1, 1\},$$

we shall get the same solution, as the following output shows.

p	q	x	y	E	3rd moment test
1	7	-3.4580	-0.0774	34.0000	$-$
1	7	2.4580	-0.9226	38.9161	$-$
2	6	-2.4365	0.1455	35.7460	$-$
2	6	1.4365	-1.1455	39.7460	$-$
3	5	-1.9434	0.3660	37.6603	$-$
3	5	0.9434	-1.3660	39.6603	$-$
4	4	-1.6180	0.6180	38.9443	$+$
4	4	0.6180	-1.6180	38.9443	$+$

Note that the last two (equivalent) lines pass the 3rd moment test. Although we get the same solution, the conclusion is less clear since we have solutions with higher energy.

7 Conclusion

The material presented in this paper shows how one might look for extremal graphs using tools from calculus. According to this approach, graphs with extremal energy "should" have a small number of distinct eigenvalues. However, the discrete nature of the problem often prevents the expected "nice" solutions from existing. In many cases, candidates other than the theoretically optimal solution must be considered. However, even if the techniques in this paper do not directly yield an extremal graph, they can also be used to guide a search for an extremal graph.

One can say that results by J.H. Koolen and V. Moulton [7] and V. Nikiforov [10] give a solution of the maximal energy problem in an asymptotic sense. As far as we know at the present, a small number of distinct eigenvalues in extremal graphs appears rarely (complete graphs for $n \leq 7$

and strongly regular graphs for $n = 10$ and $n = 4\tau^2$). Our results for $n = 8, 9, 10, 11, 12$ show that, at least for moderate values of n, the structure of maximal graphs could vary unexpectedly. Having in mind the fact that paths are maximal energy trees, such effects also appear in some form for large values of n.

It remains open whether it will be possible to describe maximal energy graphs in a better way using new approaches.

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A Mathematica Program

```
possibleEvals[numvertices_Integer, numedges_Integer, knownevals_List] :=
 Block[{eq, p, q, x, y, en},
   eq := {p + q == numvertices - Length[knownevals],
       p*x + q*y == -(Plus @@ knownevals),
       p*x^2 + q*y^2 ==
      2*numedges - (Plus @@ (knownevals^2))}; Print[ InputForm[eq]];
   Table[{p, q, x, y,  p*Abs[x] + q*Abs[y] + Plus @@ (
             Abs[knownevals]), (p*x^3 + q*
               y^3 + (Plus @@ (knownevals^3)))/6} /.
         Solve[eq // Append[#, p == i] &, {p, q, x, y}], {i, 1,
            Ceiling[(numvertices - Length[knownevals] - 1)/2]}] //
      Flatten[#, 1] &]
```

B SAGE Program

```
def possible_evals(num_vertices, num_edges, known_evals):
    # Make x and y variables
    var('x, y')
    upper_bound=ceil((1/2)*(num_vertices - len(known_evals) - 1))
```

```
for p in [1..upper_bound]:
    q = num_vertices - len(known_evals) - p
    solutions = solve([p*x + q*y == -sum(known_evals), \
      p*x^2 + q*y^2 == 2*num_edges - sum([i^2 for i in known_evals])], \
      x,y, solution_dict=True)
    for s in solutions:
        energy = p*abs(s[x]) + q*abs(s[y]) \
                 + sum([abs(e) for e in known_evals])
        third_moment_test = (1/6)*(p*s[x]^3 + q*s[y]^3 \
                                   + sum([e^3 for e in known_evals]))
        print "%d, %d, %f, %f, %f, %f"%(p, q, s[x], s[y], \
                                        energy, third_moment_test)
```