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THREE EXAMPLES OF A GROUND-BREAKING IMPACT OF THE VARIABLE NEIGHBORHOOD SEARCH ON INVESTIGATIONS IN GRAPH THEORY[1]

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Dedicated to Professor Pierre Hansen

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A b s t r a c t. The well known computer package AUTOGRAPHIX (*AGX*) *uses the variable neighborhood search to solve extremal problems in graph theory. We describe how AGX, in its very first application* (*cf. G. Caporossi, et al.* [*J. Chem. Inform. Comp. Sci.* **39** (1999), 984–996]*), has influenced substantially the study of graph energy. AGX helped very much in creating the spectral graph theory based on the signless Laplacian (see D. Cvetković, et al.* [*Publ. Inst. Math.* (*Beograd*) **81 (95)** (2007), 11–27]) *and created some non-trivial conjectures on the largest eigenvalue of a graph (see M. Aouchiche, et al.* [*Europ. J. Oper. Res.* **191** (3) (2008), 661–676]).

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1. *Introduction*

Let G be a simple graph with n vertices. The characteristic polynomial $x \mapsto \det(xI - A)$ of a $(0,1)$-adjacency matrix A of G is called the *characteristic polynomial of G* and denoted by $P_G(x)$. The eigenvalues of A (i.e., the zeros of $\det(xI-A)$) and the spectrum of A (which consists of the n eigenvalues) are also called the *eigenvalues* and the *spectrum* of G, respectively. The eigenvalues of G are usually denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$; they are real because A is symmetric. We shall assume that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and use the notation $\lambda_i = \lambda_i(G)$ for $i = 1, 2, \ldots, n$. The largest eigenvalue is also called the *index* of the graph.

The eigenvalues of A are the numbers λ satisfying $Ax = \lambda x$ for some non-zero vector $x \in I\!R^n$. Each such vector x is called an *eigenvector* of the matrix A (or of the labelled graph G) belonging to the eigenvalue λ.

Other kinds of graph eigenvalues and eigenvectors will be considered in Section 3.

As usual, K_n, C_n and P_n denote respectively the *complete graph*, the *cycle* and the *path* on n vertices. Further, $K_{m,n}$ denotes the *complete bipartite* graph on $m + n$ vertices.

The well known computer package AutoGraphiX (AGX) [6] uses the variable neighborhood search [25] to solve extremal problems in graph theory.

We describe how AGX, in its very first application [5], has influenced substantially the study of graph energy.

AGX helped very much in creating the spectral graph theory based on the signless Laplacian [14] and created some non-trivial conjectures on the largest eigenvalue of a graph [2].

Papers [5] and [2] belong to a series of over twenty papers with a common subtitle *Variable neighborhood search for extremal graphs* [3], while [14] is outside the series but in the same spirit[2]. All three papers had a ground-breaking impact on the corresponding subjects.

Next three sections are devoted to these three cases.

2. *Case 1: Graph energy*

The energy of a graph is the sum of absolute values of eigenvalues of the adjacency matrix of the graph. This definition was given by Ivan Gutman in 1978 [21]. Motivation came from theoretical chemistry but the intention was to initiate mathe-

[2] The paper [14] contains the following acknowledgement: We are grateful to P. Hansen who accepted our challenge to create some conjectures related to signless Laplacian eigenvalues using the programming package AGX, and to his collaborator M. Aouchiche whose experiments led to the formulation of the conjectures.

matical studies of this graph invariant. No significant work on this subject appeared in about next twenty years.

As stated a little bit mysteriously in Preface of [27], "sometime around the turn of the century, a dramatic change occurred, and graph energy started to attract the attention of a remarkably large number of mathematicians, all over the globe". The author will offer below his explanation of this phenomenon. Anyhow, the number of published papers on graph energy is nowadays of order of several hundred. Only in years 2008-2011 the average number of such papers was around 50 per year.

The energy is a non-smooth function and this fact, together with a discrete character of the underlying structure (graphs), makes it difficult, but also challenging, to study problems which appear. For example, the authors of [27] emphasize, as they call, Grand Open Problem (see p.192) to characterize graphs on n vertices with maximal energy. For $n = 4k^2$, k integer, extremal graphs should be strongly regular with parameters

$$(n, (n + \sqrt{n})/2, (n + \sqrt{n})/4, (n + \sqrt{n})/4)$$

if they exist [28]. It has been proved in [22] that such graphs exist for $n = 4, 16, 36$ and they are unique while for $n = 64, 100, 144$ these extremal graphs are not unique.

Note that strongly regular graphs have three distinct eigenvalues. In general, tools from calculus suggest that extremal graphs should have a small number of distinct eigenvalues but then the discrete structure of graphs prevents to find solution: simply – desired graphs do not exist [11].

In our opinion the paper [5] (reference [53] in the book [27]) had an essential influence on the further development of the subject[3], as already stated in our review [9]. This paper offered several conjectures on graph energy obtained by the use of the computer package AutoGraphiX for finding extremal graphs with respect to given graph invariants.

Among other things, a conjecture on unicyclic graphs with maximal energy (Conjecture 7.6 on p. 153 in the book) attracted much attention. The conjecture was difficult to prove (22 pages in the book). This conjecture was unusual and attractive for a mathematician. While a mathematician (perhaps not a chemist) would expect that

[3] The story behind the publication of this paper is as follows. I met Professor Pierre Hansen at an International Colloquium for Graph Theory in April 1997 in Dornföld a.d. Heide, Germany. The colloquium was dedicated to H. Sachs on the occasion of his 70-th birthday. P. Hansen was presenting his AutoGraphiX system. Since there was no experience with this system, I suggested to Hansen some extremal eigenvalue problems with trees with known solutions as first test examples. The test was successful and Hansen invited me in March 1998 to visit his institut in Montreal to work with AGX. I new that there had been no results on graph energy for many years, that it was difficult for a human to guess conjectures about it and that the existence of a new package AGX is a great opportunity to obtain conjectures. When AGX really produced very interesting and unexpected conjectures, we immediately contacted Ivan Gutman and this led, after some additional work, to publication of [5].

the cycle is extremal, the computer found that, with a finite number of exceptions, the graph consisting of a hexagon with an appended path is extremal.

The paper [5] established that among graphs on 10 vertices maximal energy has a strongly regular graph (complement of the Petersen graph). This attracted researchers working in the area of strongly regular and related graphs and we now have the Koolen-Moulton upper bound [28] for the energy of graphs with n vertices. The order of magnitude in this bound ($n^{2/3}$) was numerically predicted in [5].

3. *Case 2: Inequalities for signless Laplacian eigenvalues*

By a spectral graph theory we understand, in an informal sense, a theory in which graphs are studied by means of the eigenvalues of some graph matrix M. This theory is called M*–theory*. Hence, there are several spectral graph theories (for example, the one based on the adjacency matrix, then based on the Laplacian, etc.). In that sense, the common title "Towards a spectral theory of graphs based on the signless Laplacian" of the papers [15], [16], [17] indicates the intention to build such a spectral graph theory (the one which uses the signless Laplacian without explicit involvement of other graph matrices).

Recall that, given a graph, the matrix $Q = D + A$ is called the *signless Laplacian*, where A is the adjacency matrix and D is the diagonal matrix of vertex degrees. The matrix $L = D - A$ is known as the *Laplacian* of G.

We shall start with some definitions related to a general M–theory.

Let G be a simple graph with n vertices, and let M be a real symmetric matrix associated to G. The characteristic polynomial $\det(xI - M)$ of M is called the *M–characteristic polynomial* (or *M–polynomial*) of G and is denoted by $M_G(x)$. The eigenvalues of M (i.e., the zeros of $\det(xI-M)$) and the spectrum of M (which consists of the n eigenvalues) are also called the *M–eigenvalues of G* and the *M–spectrum of* G, respectively. The M–eigenvalues of G are real because M is symmetric, and the largest eigenvalue is called the *M–index* of G.

In particular, if M is equal to one of the matrices A, L and Q (associated to a graph G on n vertices), then the corresponding eigenvalues (or spectrum) are called the A–eigenvalues (or A–spectrum), L–eigenvalues (or L–spectrum) and Q–eigenvalues (or Q–spectrum), respectively. Throughout the paper, these eigenvalues will be denoted by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ and $q_1 \geq q_2 \geq \cdots \geq q_n$, respectively. They are the roots of the corresponding characteristic polynomials $P_G(x) = \det(xI - A)$, $L_G(x) = \det(xI - L)$ and $Q_G(x) = \det(xI - Q)$ (note, $P_G(x)$ stands for $A_G(x)$). The largest eigenvalues, i.e. λ_1, μ_1 and q_1, are called the A–index, L–index and Q–index (of G), respectively.

Together with Q–theory we shall frequently consider the relevant facts from A–

theory and L–theory as mostly developed spectral theories and therefore useful in making comparisons between theories.

There are several ways to establish inequalities for Q–eigenvalues. This area of investigation is very promising like is the case of the other spectral theories.

Paper [14] is devoted to inequalities involving Q–eigenvalues. It presents 30 computer generated conjectures in the form of inequalities for Q–eigenvalues. The conjectures were obtained by the system AGX and the paper [14] contributed substantially in building the spectral graph theory based on the signless Laplacian.

Conjectures that are confirmed by simple results already recorded in the literature, explicitly or implicitly, are identified. Some of the remaining conjectures have been resolved by elementary observations; for some quite a lot of work had to be invested. The conjectures left unresolved appear to include some difficult research problems.

We shall present here, following the paper [15] just a part of many important results obtained by considering the generated conjectures. See also [14] and [17].

One of difficult conjectures (Conjecture 24) has been confirmed in [7] by a long sequence of lemmas. The corresponding result reads:

Theorem 3.1. *The minimal value of the least Q–eigenvalue among connected non–bipartite graphs with prescribed number of vertices is attained for the odd–unicyclic graph obtained from a triangle by appending a hanging path.*

Many of the inequalities contain eigenvalues of more than one graph matrix. In particular, largest eigenvalues λ_1, μ_1 and q_1 of matrices A, L and Q, respectively, satisfy the following inequalities:

$$\mu_1 \leq q_1, \quad 2\lambda_1 \leq q_1.$$

First equality holds if and only if the graph is bipartite. See [14] for references (Conjectures 10 and 11).

These inequalities imply that any lower bound on μ_1 is also a lower bound on q_1 and that doubling any lower bound on λ_1 also yields a valid lower bound on q_1. Similarly, upper bounds on q_1 yield upper bounds on μ_1 and λ_1. Paper [32] checks whether known upper bound on μ_1 hold also for q_1 and establishes that many of them do hold.

Best upper bounds for q_1 under some conditions are given in an implicit way by the following two theorems. First we need a definition.

A graph G with the edge set E_G is called a *nested split graph*[4] if its vertices can be ordered so that $jq \in E_G$ implies $ip \in E_G$ whenever $i \leq j$ and $p \leq q$.

The following theorem can be proved in the same way as the corresponding result in A–theory [13].

[4] This term was used in [14] with an equivalent definition. The present definition is used in [12], where the graphs in question were called graphs with a *stepwise* adjacency matrix.

Theorem 3.2. *Let G be a graph with fixed numbers of vertices and edges, with maximal Q–index. Then G does not contain, as an induced subgraph, any of the graphs: $2K_2$, P_4 and C_4. Equivalently, G is a nested split graph.*

Moreover, we also have [13]:

Theorem 3.3. *Let G be a connected graph with fixed numbers of vertices and edges, with maximal Q–index. Then G does not contain, as an induced subgraph, any of the graphs: $2K_2$, P_4 and C_4. Equivalently, G is a nested split graph.*

Theorems 3.2 and 3.3 have been announced in [13] and complete proofs appear in [14]. The result has been repeated indepedently in [35]. In particular, by Theorem 3.3 we easily identify the graphs with maximal Q–index within trees, unicyclic graphs and bicyclic graphs (of fixed number of vertices). Namely, each of these sets of graphs has a unique nested split graph (see [14]). The result for bicyclic graphs has been again indepedently rediscovered in [18].

We see that both the A–index and Q–index attain their maximal values for nested split graphs. The question arises whether these extremal nested split graphs are the same in both cases. For small number of vertices this is true as existing graph data show. However, among graphs with $n = 5$ vertices and $m = 7$ edges there are two graphs (No. 5 and No. 6 for $n = 5$ in Appendix of [13]) with maximal Q–index while only one of them (No. 5) yields maximal A–index. In fact, for any $n \geq 5$ and $m = n + 2$ there are two graphs with a maximal Q–index [35].

In the next theorem we demonstrate another use of Theorem 3.3 by providing an analogue of Hong's inequality from A–theory (see [26]) to Q–theory.

Theorem 3.4. *Let G be a connected graph on n vertices and m edges. Then*

$$q_1(G) \leq \sqrt{4m + 2(n-1)(n-2)}.$$

The equality holds if and only if G is a complete graph.

The proof appears in [15].

Next one can prove an inequality relating the algebraic connectivity (the second smallest L–eigenvalue) and the second largest Q-eigenvalue of a graph.

Theorem 3.5. *Let a be the second smallest L–eigenvalue and q_2 the second largest Q–eigenvalue of a graph G with n $(n \geq 2)$ vertices. We have $a \leq q_2 + 2$ with equality if and only if G is a complete graph.*

The proof appears in [15].

Theorem 3.5 confirms Conjecture 19 of [14].

We can treat in a similar way Conjecture 20 of [14] as well.

Theorem 3.6. *Let a be the second smallest L–eigenvalue and q_2 the second largest Q–eigenvalue of a non–complete graph G with n $(n \geq 2)$ vertices. We have $a \leq q_2$.*

The proof appears in [15].

The question of the equality in Theorem 3.6. remains unsolved.

A new set of conjectures involving the largest Q–eigenvalue appears in [23]. The Q-index is considered in connection with various structural invariants, such as diameter, radius, girth, independence and chromatic number, etc. Out of 152 conjectures, generated by computer (i.e. the system AGX), many of them are simple or proved in [23], so that only 18 remained unsolved. An additional conjecture of this type has been resolved in [24]; it is proved that $q_1(G) \leq 2n(1 - 1/k)$, where k is the chromatic number, thus improving an analogous inequality for the A-index (cf. [10], p. 92).

4. *Case 3: Some difficult conjectures on the largest eigenvalue*

The conjectures from the paper [2] are related to the maximal value of the irregularity and spectral spread in n-vertex graphs and to a Nordhaus-Gaddum type upper bound for the index. None of the conjectures has been resolved so far. We present partial results and provide some indications that the conjectures are very hard.

Let G be a graph with n vertices and m edges. Let $\lambda_1(G) = \lambda_1, \lambda_n(G) = \lambda_n$ be the largest and the least eigenvalue of G respectively. Let $\lambda_1(\overline{G}) = \overline{\lambda}_1$. If G is connected, there is a positive eigenvector belonging to λ_1. The unique positive eigenvector of λ_1 is the *principal* eigenvector of G.

The difference between the index and the average vertex degree is called the *irregularity* of a graph [8].

The quantity $\lambda_1 - \lambda_n$ is called the *spectral spread* of the graph.

The *union* of (disjoint) graphs G and H is denoted by $G \cup H$, while mG denotes the union of m disjoint copies of G.

The *join* $G \nabla H$ of (disjoint) graphs G and H is the graph obtained from G and H by joining each vertex of G with each vertex of H.

We shall continue by giving definitions of some specific notions.

A *complete split graph* with parameters n, q $(q \leq n)$, denoted by $CS(n, q)$, is a graph on n vertices consisting of a clique on q vertices and a stable set on the remaining $n - q$ vertices in which each vertex of the clique is adjacent to each vertex of the stable set.

A *fanned complete split graph* with parameters n, q, t $(n \geq q \geq t)$, denoted by $FCS(n, q, t)$, is a graph (on n vertices) obtained from a complete split graph $CS(n, q)$ by connecting a vertex from the stable set by edges to t other vertices of the stable set.

A *pineapple* with parameters n, q $(q \leq n)$, denoted by $PA(n, q)$, is a graph on n vertices consisting of a clique on q vertices and a stable set on the remaining $n - q$ vertices in which each vertex of the stable set is adjacent to a unique vertex of the clique.

A *fanned pineapple of type* i $(i = 1, 2)$ with parameters n, q, t $(n \geq q \geq t)$, denoted by $FPA_i(n, q, t)$, is a graph (on n vertices) obtained from a pineapple $PA(n, q)$ by connecting a vertex from the stable set by edges to t vertices of the

1) clique, with $0 \leq t \leq q - 2$, for $i = 1$,

2) stable set, with $0 \leq t < n - q$, for $i = 2$.

We have $FPA_i(n, q, 0) = PA(n, q)$ for $i = 1, 2$.

The following conjectures related to the index of a graph have been formulated after some experiments with the system AutoGraphiX (AGX).

Conjecture 4.1. *The most irregular connected graph on* n $(n \geq 10)$ *vertices is a pineapple* $PA(n, q)$ *in which the clique size* q *is equal to* $\lceil \frac{n}{2} \rceil + 1$.

This assertion has been established by AGX for $n = 10, 11, \ldots, 17$. For smaller values of n the maximal graph is again a pineapple (reduced to a star for $n = 5, 6, 7$).

Conjecture 4.2. *Given* n*, the maximal value of the spectral spread of a graph on* n *vertices is obtained for a complete split graph* $CS(n, q)$ *with an independent set of size* $n - q = \lceil \frac{n}{3} \rceil$.

Conjecture 4.3. *Maximal graphs on* n *vertices for the function* $\lambda_1 + \overline{\lambda}_1$ *are complete split graphs* $CS(n, q)$ *with the clique size equal or close to* $n/3$.

More precisely, for any simple graph G, with complement $\bar{G}$, spectral radius $\lambda_1(G)$ and n vertices we have

$$\lambda_1(G) + \lambda_1(\bar{G}) \leq \frac{4}{3}n - \frac{5}{3} - \begin{cases} f_1(n) & if \quad n \pmod 3 \equiv 1, \\ 0 & if \quad n \pmod 3 \equiv 2, \\ f_2(n) & if \quad n \pmod 3 \equiv 0, \end{cases}$$

where

$$f_1(n) = \frac{3n - 2 - \sqrt{9n^2 - 12n + 12}}{6} \quad \text{and} \quad f_2(n) = \frac{3n - 1 - \sqrt{9n^2 - 6n + 9}}{6}.$$

This bound is sharp and attained if and only if G or $\bar{G}$ is a complete split graph with an independent set on $\lfloor \frac{n}{3} \rfloor$ vertices (and also on $\lceil \frac{n}{3} \rceil$ vertices if $n \pmod 3 \equiv 2$).

We shall describe in some detail the use of AGX in formulating Conjecture 4.3.

Additional experiments have shown that maximal graphs for $\lambda_1 + \overline{\lambda}_1$ for given n and m are complete split graphs or fanned complete split graphs with a few exceptions.

When looking for extremal graphs with the system AutoGraphiX (AGX), using the variable neighborhood search metaheuristic, we defined the objective function as $\lambda_1(G) + \lambda_1(\bar{G})$ to be maximized over the class of all graphs having from 4 to 24 vertices. To be coherent in our investigations, we required the graph G, but not necessarily its complement $\bar{G}$, to be connected. This constraint is without loss of generality because of the fact that at least one of the complementary graphs G and $\bar{G}$ is connected.

For a fixed number of vertices n, the extremal graph G is composed of a clique on q vertices and a stable set with s vertices in which every vertex is connected to all vertices of the clique. When we observed the values of q and s for different graphs, we found the following:

$$q = \begin{cases} \lfloor \frac{n}{3} \rfloor & if \quad n \,(\mathrm{mod}\ 3) \equiv 1 \\ \frac{n}{3} & if \quad n \,(\mathrm{mod}\ 3) \equiv 0 \end{cases} \quad \text{and} \quad s = \begin{cases} \lceil \frac{2n}{3} \rceil & if \quad n \,(\mathrm{mod}\ 3) \equiv 1 \\ \frac{2n}{3} & if \quad n \,(\mathrm{mod}\ 3) \equiv 0. \end{cases}$$

While the experiments show regularity for the cases $n \pmod 3 \equiv 0$ and $n \pmod 3 \equiv 1$, it was not the case when $n \,(\mathrm{mod}\ 3) \equiv 2$. Sometimes we have $q = \lfloor \frac{n}{3} \rfloor$ and $s = \lceil \frac{2n}{3} \rceil$ and other times, we have $q = \lceil \frac{n}{3} \rceil$ and $s = \lfloor \frac{2n}{3} \rfloor$. We decided to examine the two cases interactively on *AGX* for every n, and we observed that the objective function has the same value in both cases $\big(q = \lfloor \frac{n}{3} \rfloor$ or $q = \lceil \frac{n}{3} \rceil\big)$.

AGX did not find any conjecture on the relation between the objective function $\lambda_1(G) + \lambda_1(\bar{G})$ and the number of vertices when using all the presumably extremal graphs obtained by AGX. But when we separated the set of graphs into three subsets, with $n \pmod 3 \equiv 0$ for the first subset, $n \pmod 3 \equiv 1$ for the second one and $n \pmod 3 \equiv 2$ for the third one, *AGX* did not find anything about the two first subsets but suggested the following linear relation for the third one ($n \pmod 3 \equiv 2$)

$$\lambda_1(G) + \lambda_1(\bar{G}) = \frac{4}{3}n - \frac{5}{3}.$$

Conjecture 4.3 suggests a result of Nordhaus-Gaddum type. Such results have a long history.

In 1956, Nordhaus and Gaddum [30] proved that

$$2\sqrt{n} \leq \chi(G) + \chi(\bar{G}) \leq n + 1$$

and

$$n \leq \chi(G) \cdot \chi(\bar{G}) \leq \frac{(n+1)^2}{4}.$$

Finck [19] showed that these bounds were sharp (taking ceilings if necessary) and characterized extremal graphs. Similar bounds were obtained for a large number of graph invariants by a variety of authors. Let $i(G)$ denote a graph invariant, *i.e.*, a function defined for all graphs and whose value is independent of vertex or edge labelling. Classical Nordhaus-Gaddum relations are of the following form:

$$l_1(n) \leq i(G) + i(\bar{G}) \leq u_1(n)$$

and

$$l_2(n) \leq i(G) \cdot i(\bar{G}) \leq u_2(n)$$

in more general form, the lower and upper bounding functions may depend on several variables.

Nosal [31] and Amin and Hakimi [1] independently proved that

$$n - 1 \leq \lambda_1(G) + \lambda_1(\bar{G}) \leq \sqrt{2}(n-1).$$

The lower bound is attained if and only if the graph is regular.

It is proved in [29] that

$$\lambda_1(G) + \lambda_1(\bar{G}) \leq \sqrt{\Big(2 - \frac{1}{k} - \frac{1}{\bar{k}}\Big) n(n-1)},$$

where k and $\bar{k}$ are the size of a maximal clique in G and $\bar{G}$ respectively.

Little can be found in the literature concerning the spectral spread of a graph. All graphs whose spectral spread does not exceed 4 are determined in [33]. The spectral spread of unicyclic graphs has been studied in [36].

However, Conjecture 4.2 did appear in the literature (cf. [20]) but remained unsolved. It is noted in [20] that the conjecture has been verified by computer for graphs up to 9 vertices.

The difficulty in proving Conjectures 4.2 and 4.3 is that we have almost no lemmas on the behavior of the corresponding invariant under local graph transformations. Experiments with computer packages such as GRAPH, newGRAPH and AGX would be useful in producing conjectures for such lemmas (e.g. adding an edge, rotating an edge etc.). However, for the irregularity of a graph (involved in Conjecture 4.1) we do have such lemmas (see Section 6 of [2]).

The common characteristic of the three conjectures is that the graph invariant involved is the sum or the difference of two invariants which behave differently when varying some parameters (e.g. the number of edges).

See the monograph [34] for some recent results on the three conjectures which remained unresolved.

5. *Conclusion*

We have described three examples of a ground-breaking impact of the variable neighborhood search, implemented within the system AutoGraphiX (AGX), on investigations in graph theory, in particular, in spectral graph theory.

The paper [5] enabled a ground-breaking development of research in the area of graph energy with several hundreds of papers published as a consequence.

The paper [14] helped very much in creating the spectral graph theory based on the signless Laplacian, again with several hundreds of papers published.

The paper [2] is of somewhat different character. It provided conjectures difficult to resolve. The papers published on these conjectures are not numerous because the conjectures are really difficult.

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