THE LAPLACIAN SPECTRUM OF GRAPHS †

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Abstract. The paper is essentially a survey of known results about the spectrum of the Laplacian matrix of graphs with special emphasis on the second smallest Laplacian eigenvalue λ_2 and its relation to numerous graph invariants, including connectivity, expanding properties, isoperimetric number, maximum cut, independence number, genus, diameter, mean distance, and bandwidth-type parameters of a graph. Some new results and generalizations are added.

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1. INTRODUCTION

The Laplacian matrix of a graph and its eigenvalues can be used in several areas of mathematical research and have a physical interpretation in various physical and chemical theories. The related matrix — the adjacency matrix of a graph and its eigenvalues were much more investigated in the past than the Laplacian matrix. The reader is referred to the monographs [CDS, CDGT]. However, in the author's opinion the Laplacian spectrum is much more natural and more important than the adjacency matrix spectrum. It is the aim of this survey paper to explain where this belief comes from.

We shall use the standard terminology of graph theory, as it is introduced in most text-books on the theory of graphs (e.g., [Wi]). Our graphs are unoriented, but they may have loops and multiple edges. We also allow *weighted graphs* which are viewed as a graph which has for each pair u, v of vertices, assigned a certain *weight* a_{uv}. The weights are usually real numbers and they must satisfy the following conditions:

(i) $a_{uv} = a_{vu}, \quad v, u \in V(G)$, and

(ii) $a_{vu} \neq 0$, if and only if v and u are adjacent in G.

Usually the additional condition on the non-negativity of weights is assumed:

(iii) $a_{uv} \geq 0, \quad v, u \in V(G)$.

It will be clear from the context or otherwise explicitly specified if a graph is weighted. Unweighted graphs can be viewed as a special case of weighted graphs, by specifying, for each $u, v \in V(G)$, the weight a_{uv} to be equal to the number of edges between u and v. The matrix $A = A(G) = [a_{uv}]_{u,v \in V(G)}$, is called the *adjacency matrix* of the graph G. We shall use the same name for the matrix of weights if the graph is weighted.

Let $d(v)$ denote the degree of $v \in V(G), d(v) = \sum_u a_{uv}$, and let $D = D(G)$ be the diagonal matrix indexed by $V(G)$ and with $d_{vv} = d(v)$. The matrix $Q = Q(G) = D(G) - A(G)$ is called the *Laplacian matrix* of G. It should be noted at once that loops have no influence on $Q(G)$. The matrix $Q(G)$ is sometimes called the *Kirchhoff matrix* of G due to its role in the well-known Matrix-Tree Theorem (cf. §4) which is usually attributted to Kirchhoff. Another name, the *matrix of admittance*, comes from the theory of electrical networks (admittance = conductivity). It should be mentioned here that the rows and columns of graph matrices are indexed by the vertices of the graph, their order being unimportant. The matrix $Q(G)$ acts naturally on the vector space $\ell^2(V(G))$. For any vector $x \in \ell^2(V(G))$ we denote its coordinates by $x_v, v \in V(G)$.

Throughout the paper we shall denote by $\mu(G,x)$ the characteristic polynomial of $Q(G)$. Its roots will be called the *Laplacian eigenvalues* (or sometimes just *eigenvalues*) of G. They will be denoted by $\lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$ ($n = |V(G)|$), always enumerated in increasing order and repeated according to their multiplicity. We shall use the notation $\lambda_k(G)$ to denote the k-th smallest eigenvalue of the graph G (counting multiplicities). The letter n will always stand for the order of G, so $\lambda_n(G)$ will be the maximal eigenvalue of $Q(G)$.

Let G be a given graph. Orient its edges arbitrarily, i.e. for each $e \in E(G)$ choose one of its ends as the *initial* vertex, and name the other end the *terminal* vertex. The *oriented incidence matrix* of G with respect to the given orientation is the $|V| \times |E|$ matrix $C = [c_{ve}]$ with entries

$$c_{ve} = \begin{cases} +1, & \text{if } v \text{ is the terminal vertex of } e, \\ -1, & \text{if } v \text{ is the initial vertex of } e, \\ 0, & \text{if } v \text{ and } e \text{ are not incident.} \end{cases}$$

It is well known that

$$Q(G) = CC^{\mathrm{t}} \tag{1.1}$$

independent of the orientation given to the edges of G (cf., e.g., [Bi]). It should be noted that (1.1) immediately implies the formula (2.1) since the inner product $(Q(G)x, x)$ is equal to $(CC^{\mathrm{t}}x, x) = (C^{\mathrm{t}}x, C^{\mathrm{t}}x)$.

The Laplace differential operator Δ is one of the basic differential operators in mathematical physics. One looks for non-trivial solutions of $\Delta\phi = \lambda\phi$ on a certain region Ω. By discretizing the Laplace equation one gets the Laplacian matrix Q of the discretisized space (usually a graph). We mention that, by this correspondence, the oriented incidence matrix C, as defined above, corresponds to the gradient operator, and so (1.1) has a clear physical interpretation.

In Section 2 we review the basic spectral properties of $Q(G)$. The next section presents the results on the spectra of graphs obtained by means of some operations on graphs, including the disjoint union, Cartesian product and the join of graphs, deleting or inserting an edge, the complement, the line graph, etc. Section 4 is devoted to the renowned application of $Q(G)$, the Matrix-Tree-Theorem, which expresses the number of spanning trees of a graph in terms of its non-zero eigenvalues.

There are many problems in physics and chemistry where the Laplacian matrices of graphs and their spectra play the central role. Some of the applications are mentioned in Section 5. It is worth noting that the physical background served as the idea of a well known algorithm of W.T. Tutte [T] for testing planarity and constructing "nice" planar drawings of 3-connected planar graphs.

The second smallest Laplacian eigenvalue λ_2 plays a special role. Recently its applications to several difficult problems in graph theory were discovered (e.g., the expanding properties of graphs, the isoperimetric number, and the maximum cut problem). Section 6 presents these applications, including the relation of λ_2 to the diameter and the mean distance of a graph. In addition, a relation of λ_2 to the independence number, genus, and bandwidth-type invariants is presented. The structure of the eigenvectors corresponding to λ_2 is discussed in the next section. The last section covers a few other results on $Q(G)$ and its applications.

There are some new results in this paper. Many of them are more or less trivial and have probably been known to researchers in the field, although not published before. The results surveyed in the paper are biased by the viewpoint of the author. We apologize to all who feel that their work is missing in the references, or has not been emphasized sufficiently in the text.

2. BASIC PROPERTIES

The following properties were established by several authors [K3, V, AnM] for the case of unweighted graphs. The proofs carry over to the weighted case if all the weights are non-negative.

2.1. Theorem. Let G be a (weighted) graph with all weights non-negative. Then:

(a) $Q(G)$ has only real eigenvalues,

(b) $Q(G)$ is positive semidefinite,

(c) its smallest eigenvalue is $\lambda_1 = 0$ and a corresponding eigenvector is $(1, 1, \dots, 1)^{\mathrm{t}}$. The multiplicity of 0 as an eigenvalue of $Q(G)$ is equal to the number of components of G.

We mention that the positive semidefiniteness of $Q(G)$ follows from the next useful expression for the inner product $(Q(G)x, x)$ which holds also in the weighted case:

$$(Q(G)x, x) = \sum_{vu \in E} a_{vu}(x_v - x_u)^2 \tag{2.1}$$

Let $\lambda_1 \le \lambda_2 \le \dots \le \lambda_n$ be the eigenvalues of $Q(G)$ in increasing order and repeated according to their multiplicity. So, $\lambda_1 = 0$, and $\lambda_2 > 0$ if and only if G is connected. The following bounds for the eigenvalues are known.

2.2. Theorem. Let G be a graph of order n. Then:

(a) [F1] $\lambda_2 \le \frac{n}{n-1} \min\{d(v); v \in V(G)\}$.

(b) [AnM] $\lambda_n \le \max\{d(u) + d(v); uv \in E(G)\}$. If G is connected then the equality holds if and only if G is bipartite semiregular.

(c) [K3] If G is a simple graph then $\lambda_n \le n$ with equality if and only if the complement of G is not connected.

(d) $\sum\limits_{i=1}^{n} \lambda_i = 2|E(G)| = \sum_v d(v)$.

(e) [F1] $\lambda_n \ge \frac{n}{n-1} \max\{d(v); v \in V(G)\}$.

(f) [MM, p.168] $\lambda_n \ge \max\{\sqrt{(d(v) - d(u))^2 + 4a_{uv}^2}\,; v, u \in V(G),\, v \ne u\}$.

Let G be a (weighted) graph and $V_1 \cup V_2 \cup \ldots \cup V_k$ a partition of its vertex set. This partition is said to be *equitable* if for each $i, j = 1, 2, \ldots, k$ there is a number d_{ij} such that for each $v \in V_i$ there are exactly d_{ij} edges between v and vertices in V_j ($\sum_{u \in V_j} a_{vu} = d_{ij},\ v \in V_i$). The name equitable partition was introduced by Schwenk. There are several other terms used for the same thing (e.g., divisor [CDS], coloration, degree refinement, etc.).

2.3. Theorem. Let $V_1 \cup V_2 \cup \ldots \cup V_k$ be an equitable partition of G with parameters d_{ij} ($i, j = 1, 2, \ldots, k$), and let $B = [b_{ij}]_{i,j=1,\ldots,k}$ be the matrix defined by

$$b_{ij} = \begin{cases} -d_{ij}, & \text{if} \quad i \neq j \\ (\sum_{s=1}^{k} d_{is}) - d_{ii}, & \text{if} \quad i = j. \end{cases}$$

If λ is an eigenvalue of B then λ is also an eigenvalue of $Q(G)$.

Proof. Let $Bx = \lambda x, x = (x_1, \ldots, x_k)^{\mathrm{t}}$. Let $y = (y_v)_{v \in V(G)}$ be defined by: if $x \in V_i$ then let $y_v = x_i$. Now it is not too difficult to verify that $Q(G)y = \lambda y$. Let $v \in V_i$ be any vertex of G. Then

$$\begin{aligned}(Qy)_v = d(v)y_v - \sum_u a_{vu} y_u = (\sum_{j=1}^{k} d_{ij}) x_i - \sum_{j=1}^{k} d_{ij} x_j = \\ = (Bx)_i = \lambda x_i = \lambda y_v.\end{aligned}$$

Note. We may view $D = [d_{ij}]$ as the matrix of a weighted *directed* graph with k vertices. Then B is just its Laplacian matrix.

Let us mention briefly that equitable partitions of vertices arise in many important situations. For example, if $p\colon \tilde{G} \to G$ is a graph covering projection (in the sense of topology) then the fibres $p^{-1}(v),\ v \in V(G)$, form an equitable partition of $\tilde{G}$. The corresponding matrix B is just $Q(G)$, and this shows that the Laplacian spectrum of $\tilde{G}$ contains the spectrum of G. Many examples of equitable partitions of a graph G are obtained by taking, as the classes of a partition, the orbits of some group of automorphisms of the graph G.

3. OPERATIONS ON GRAPHS AND THE RESULTING SPECTRA

Many published works relate the Laplacian eigenvalues of graphs with the eigenvalues of graphs obtained by means of some operations on the graphs we start with. The first result is obvious.

3.1. Theorem. Let G be the disjoint union of graphs $G_1, G_2, \ldots, G_k$. Then

$$\mu(G,x) = \prod_{i=1}^{k} \mu(G_i,x).$$

Let G be a (weighted) graph and let $G' = G + e$ be the graph obtained from G by inserting a new edge e into G (possibly increasing the multiplicity of an existing edge). Then $Q(G')$ and $Q(G)$ differ by a positive semidefinite matrix of rank 1. It follows by the Courant-Weyl inequalities (see, e.g., [CDS, Theorem 2.1]) that the following is true.

3.2. Theorem. The eigenvalues of G and $G' = G + e$ interlace:

$$0 = \lambda_1(G) = \lambda_1(G') \le \lambda_2(G) \le \lambda_2(G') \le \lambda_3(G) \le \ldots \le \lambda_n(G) \le \lambda_n(G').$$

We notice that $\sum_{i=1}^{n} (\lambda_i(G') - \lambda_i(G)) = 2$ by Theorem 2.2(d), so that at least one inequality $\lambda_i(G) \le \lambda_i(G')$ must be strict.

By inserting more than one edge we may loose interlacing of the eigenvalues. Nevertheless, there is an important result on λ_2.

3.3. Theorem. Let $G = G_1 \oplus G_2$ be a factorization of a graph G. Then

(a) [F1] $\lambda_2(G) \ge \lambda_2(G_1) + \lambda_2(G_2)$.

(b) $\max\{\lambda_n(G_1), \lambda_n(G_2)\} \le \lambda_n(G) \le \lambda_n(G_1) + \lambda_n(G_2)$.

Note. In Theorem 3.3, graphs may be weighted with non-negative weights. In that case the factorization means that the uv-weight in G is the sum of the uv-weights in G_1 and G_2.

Proof. (b) $G = G_1 \oplus G_2$ means that $Q(G) = Q(G_1) + Q(G_2)$. Then

$$\lambda_n(G) = \max_{\|x\|=1} (Q(G)x, x) = \max_{\|x\|=1} [(Q(G_1)x, x) + (Q(G_2)x, x)] \leq$$
$$\leq \max_{\|x\|=1} (Q(G_1)x, x) + \max_{\|x\|=1} (Q(G_2)x, x) = \lambda_n(G_1) + \lambda_n(G_2).$$

The other inequality follows from a similar consideration.

3.4. Corollary. [F1] If G_1 is a spanning subgraph of G_2 then $\lambda_2(G_1) \leq \lambda_2(G_2)$.

Fiedler [F1] derived also a result about the Cartesian products of graphs.

3.5. Theorem. [F1] The Laplacian eigenvalues of the Cartesian product $G_1 \times G_2$ of graphs G_1 and G_2 are equal to all the possible sums of eigenvalues of the two factors:

$$\lambda_i(G_1) + \lambda_j(G_2), \qquad i = 1, \ldots, |V(G_1)|, \quad j = 1, \ldots, |V(G_2)|.$$

By applying Theorem 3.5 we can easily determine the spectrum of “lattice” graphs. The $m \times n$ lattice graph is just the Cartesian product of paths, $P_m \times P_n$. The spectrum of P_k is [AnM]

$$\ell_i^{(k)} = 4\sin^2(\frac{\pi i}{2k}), \qquad i = 0, 1, \ldots, k-1$$

so $P_m \times P_n$ has eigenvalues

$$\lambda_{i,j} = \ell_i^{(m)} + \ell_j^{(n)} = 4\sin^2(\frac{\pi i}{2m}) + 4\sin^2(\frac{\pi j}{2n}).$$

The next two results were first observed by Kel’mans [K1, K2].

3.6. Theorem. [K1, K2] If $\overline{G}$ denotes the complement of the graph G then

$$\mu(\overline{G}, x) = (-1)^{n-1} \frac{x}{n-x} \mu(G, n-x)$$

and so the eigenvalues of $\overline{G}$ are $\lambda_1(\overline{G}) = 0$, and

$$\lambda_{i+1}(\overline{G}) = n - \lambda_{n-i+1}(G), \qquad i = 1, 2, \ldots, n-1.$$

Note: Theorem 3.6 has a generalization to the weighted case, see [MP], if we define the weights of $\overline{G}$ to be $a'_{uv} = 1 - a_{uv}$ ($u \neq v$).

3.7. Corollary. [K1, K2] Let $G_1 * G_2$ denote the join of G_1 and G_2, i.e. the graph obtained from the disjoint union of G_1 and G_2 by adding all possible edges uv, $u \in V(G_1), v \in V(G_2)$. Then

$$\mu(G_1 * G_2, x) = \frac{x(x - n_1 - n_2)}{(x - n_1)(x - n_2)} \mu(G_1, x - n_2)\mu(G_2, x - n_1).$$

where n_1 and n_2 are orders of G_1 and G_2, respectively.

Let G be a simple unweighted graph. The *line graph* $L(G)$ of G is the graph whose vertices correspond to the edges of G with two vertices of $L(G)$ being adjacent if and only if the corresponding edges in G have a vertex in common. The *subdivision graph* $S(G)$ of G is obtained from G by inserting, into each edge of G, a new vertex of degree 2. The *total graph* $T(G)$ of G has its vertex set equal to the union of vertices and edges of G, and two of them being adjacent if and only if they are incident or adjacent in G.

3.8. Theorem. [K3] Let G be a d-regular simple graph with m edges and n vertices. Then

(a) $\mu(L(G), x) = (x - 2d)^{m-n}\mu(G, x)$

(b) $\mu(S(G), x) = (-1)^m(2 - x)^{m-n}\mu(G, x(d + 2 - x))$

(c) $\mu(T(G), x) = (-1)^m(d + 1 - x)^n(2d + 2 - x)^{m-n}\mu(G, \frac{x(d+2-x)}{d+1-x})$.

The part (a) of Theorem 3.8 was also obtained by Vahovskii [V]. Theorem 3.8(a) can be proved also for bipartite semiregular graphs. Recall that a graph G is (r, s)-*semiregular* if it is bipartite with a bipartition $V = U \cup W$ such that all vertices in U have degree r and all vertices in W have degree s.

3.9. Theorem. If G is a simple (r, s)-semiregular graph then

$$\mu(L(G), x) = (-1)^n (x - (r+s))^{m-n} \mu(G, r+s-x).$$

Proof. Orient the edges of G in the direction from U to W ($U \cup W$ is a semiregular bipartition) and let C be the oriented incidence matrix of G with respect to this orientation. Then

$$CC^{\mathrm{t}} = Q(G) \qquad \text{and} \qquad C^{\mathrm{t}}C = 2I + A(L(G)).$$

The line graph of an (r, s)-semiregular graph is $(r+s-2)$-regular, hence $Q(L(G)) = (r+s-2)I - A(L(G))$. It is well-known that the matrices CC^{t} and $C^{\mathrm{t}}C$ have the same eigenvalues with the exception of the possible eigenvalue 0. It follows that $\mu(G, x)$ and the characteristic polynomial of $(r+s)I - Q(L(G))$ have the same non-zero roots (including their multiplicities). The proof is finished by observing that the difference between the dimensions of $Q(L(G))$ and $Q(G)$ is $m - n$ and the fact that the leading coefficient of the characteristic polynomial is equal to 1.

Note. a) If G is (r, s)-semiregular then $\lambda_n(G) = r + s$ and this eigenvalue corresponds, by the formula of Theorem 3.9, to the eigenvalue 0 of $\mu(L(G), x)$.

b) Let $\varphi(.,.)$ denote the characteristic polynomial of the adjacency matrix of the graph. It is clear from the proof of Theorem 3.9 that $\varphi(L(G), x) = (x+2)^{m-n} \mu(G, x+2)$ for any bipartite graph G.

Subdivision graphs, with many vertices subdividing each edge of the original graph, and their spectra are particularly important in the study of thermodynamic properties of crystalline solids (cf. §5). This practical problem led B.E. Eichinger and J.E. Martin [EM] to devise an algorithm for computing the Laplacian eigenvalues of a subdivided graph by applying numerical linear algebraic methods only to the matrix of the unsubdivided graph.

4. THE MATRIX-TREE-THEOREM

The most renowned application of the Laplacian matrix of a graph is in the well-known Matrix-Tree-Theorem. This result is usually attributed to Kirchhoff [Ki].

4.1. Theorem. (Matrix-Tree-Theorem). Let u, v be vertices of a graph G, and let $Q_{(uv)}$ be the matrix obtained from $Q(G)$ by deleting the row u and the column v. The absolute value of the determinant of $Q_{(uv)}$ is equal to the number of spanning trees $\kappa(G)$ of the graph G.

4.2. Corollary. The number $\kappa(G)$ of spanning trees of the graph G of order n is equal to

$$\frac{1}{n}(-1)^{n-1}\,\mu'(G,0) = \frac{1}{n}\lambda_2(G)\lambda_3(G)\cdots\lambda_n(G).$$

A generalization of the Matrix-Tree-Theorem was obtained by Kel'mans [K3] who gave a combinatorial interpretation to all the coefficients of $\mu(G,x)$ in terms of the numbers of certain subforests of the graph. This result has been obtained even in greater generality (for weighted graphs) by Fiedler and Sedláček [FS].

4.3. Theorem. [FS, K3] If $\mu(G,x) = x^n + c_1x^{n-1} + \cdots + c_{n-1}x$ then

$$c_i = (-1)^i \sum_{\substack{S \subset V \\ |S|=n-i}} \kappa(G_S)$$

where $\kappa(H)$ is the number of spanning trees of H, and G_S is obtained from G by identifying all points of S to a single point.

In [K4] graphs are compared by their polynomial $\mu(G,x)$ with application to the number of spanning trees. Kel'mans and Chelnokov [KC] consider the problem of determining the graphs with extreme number of spanning trees (minimal, or maximal) in the family of graphs with a given number of vertices and edges. They make use of Corollary 4.2. Constantine [Co] further generalizes the results of [KC].

5. PHYSICAL AND CHEMICAL APPLICATIONS

The Laplace differential operator Δ is one of the basic differential operators in mathematical physics. There are two boundary problems connected with this operator. In each of them one has to look for non-trivial solutions of $\Delta\phi = \lambda\phi$ on Ω. If we add the boundary condition $\phi_{|\partial\Omega} = 0$ we get the *Dirichlet problem.* The same equation with the *Neumann condition* at the boundary describes the vibration of a membrane which does not have its boundary fixed. The same two problems have been studied on Riemannian manifolds. It also makes sense to consider Riemannian manifolds without boundary, in which case there is no distinction between both problems (see, e.g. [Cha]).

The discretization of these problems gives rise to the Laplacian matrix of a graph (possibly infinite) and the eigenvalue problem for this matrix.

The first problem we mention is the vibration of a membrane. It is described by the Laplace equation

$$\Delta z = -\lambda z, \quad z = 0 \text{ on } \Gamma \tag{5.1}$$

where Γ is a simple closed curve in the z-plane. Discrete analogue of Δ is the Laplacian matrix of a graph which discretizes the region where the equation (5.1) is studied, cf. [CDS, p. 257].

Fisher [Fi] discusses a discrete model of a vibrating membrane where interaction occurs only between neighbouring atoms (vertices of a graph). The discretization of the vibration of a membrane in this model leads to the Laplacian matrix of the graph with its eigenvalues corresponding to the characteristic frequencies of the membrane. (It seems that the author of [Fi] realizes, because of the regularity of his "lattice" graphs, the connection with adjacency matrix eigenvalues, and addresses the general problem to $A(G)$.) The Laplacian problem on graphs in this interepretation determines the so-called *combinatorial drum* [CDS, p.256]. It means vibrating of a drum membrane without boundary.

Viewing a graph as a system of vertices joined by elastic springs representing its edges, and observing that a kinematic system which vibrates in the xy-plane tends to its equilibrium (stationary) state, led W.T. Tutte [T] to a very interesting algorithm for convex straight-line embeddings of 3-connected planar graphs in the plane. First, one has to select a non-separating induced cycle C of the given 3-connected graph G. Let $(x_1, y_1), (x_2, y_2), \ldots, (x_k, y_k)$ be the vertices of a convex k-gon in the plane where k is the length of C. These points will be the coordinates of vertices of C in the constructed embedding. There are unique solutions x, y of

$$Q(G)x = x^\circ \quad \text{and} \quad Q(G)y = y^\circ \tag{5.2}$$

where the components of $x = (x_v)_{v \in V}$ corresponding to vertices on C are equal to their coordinates x_i, and the other components of x are unknowns. The vector x° on the right side of (5.2) has all coordinates corresponding to vertices not on C equal to 0 and the others unknown. Similar holds for y and y°. It turns out [T] that the solution x, y of (5.2) determines the coordinates of a planar convex, straight-line embedding of G if and only if G is planar.

The Laplacian matrix appears also in the theory of electrical currents and flows — the incidence matris C and $Q = CC^{\mathrm{t}}$ can be found in the famous Kirchhoff laws. As a reference we give the classical Kirchhoff's paper [Ki].

C. Maas showed in [Ma] that the Laplacian eigenvalues of the underlying graph determine the kinematic behaviour of a liquid flowing through a system of communicating pipes. It turns out that the second smallest eigenvalue λ_2 (see also §6) determines the basic behaviour of the flow (e.g., whether the flow is of periodic, or aperiodic type).

Let G be a graph representing a system of beads as vertices and edges representing the mutual interactions between these beads. Then the potential, or the kinematic energy of such a system is a quadratic form which can be expressed (cf. (2.1)) by the use of the Laplacian matrix of G. Many related physical quantities have the same relation to $Q(G)$. Eichinger, *et al.* [E1, E2, E3, E4, EM] for example showed that the eigenvalues of the Laplacian matrix of a molecular graph determine the distribution function of the so-called radius of gyration of the molecule, and that the non-zero eigenvalues and their eigenvectors can be used efficiently to compute the scattering functions for Gaussian molecules. See [GS] for some additional references. It is worth mentioning that the asymptotic behaviour of the distribution function of the radius of gyration of a molecule depends mostly upon the magnitude and multiplicity of λ_2 [E1].

6. λ_2 - THE ALGEBRAIC CONNECTIVITY OF GRAPHS

The second smallest Laplacian eigenvalue λ_2 of graphs is probably the most important information contained in the spectrum of a graph. This eigenvalue is related to several important graph invariants, and it has been extensively investigated. Most of the results are consequences of the well-known Courant-Fischer principle which states that

$$\lambda_2(G) = \min_{\substack{x \perp \mathbf{1} \\ x \neq \mathbf{0}}} \frac{(Q(G)x, x)}{(x, x)} \tag{6.1}$$

where $\mathbf{0} = (0, 0, \ldots, 0)^{\mathrm{t}}$, and $\mathbf{1} = (1, 1, \ldots, 1)^{\mathrm{t}}$ is an eigenvector of $\lambda_1 = 0$. Fiedler [F2] obtained another espression for λ_2.

6.1. Proposition. [F2] Let G be a weighted graph with non-negative weights a_{uv}. Then

$$\lambda_2(G) = 2n \min_{x \in \Phi} \frac{\sum\limits_{uv \in E(G)} a_{uv}(x_u - x_v)^2}{\sum\limits_{u \in V} \sum\limits_{v \in V} (x_u - x_v)^2} \tag{6.2}$$

where Φ is the set of all non-constant vectors $x \in \ell^2(V)$.

It can be shown easily, using the fact that $\lambda_n(G) = |V(G)| - \lambda_2(\bar{G})$, that a similar formula holds for the maximal eigenvalue of a graph:

$$\lambda_n(G) = 2n \max_{x \in \Phi} \frac{\sum\limits_{uv \in E(G)} a_{uv}(x_u - x_v)^2}{\sum\limits_{u \in V} \sum\limits_{v \in V} (x_u - x_v)^2} \tag{6.2$'$}$$

Fiedler [F1, F3] calls the number $\lambda_2(G)$ the *algebraic connectivity* of the graph G. This is influenced by its relation to the classical connectivity parameters of the graph — the *vertex connectivity* $\nu(G)$ and the *edge connectivity* $\eta(G)$.

6.2. Theorem. [F1] Let G be a graph of order n and with maximal valency $\Delta(G)$, and denote by $\omega = \frac{\pi}{n}$. Then

(a) $\lambda_2(G) \leq \nu(G) \leq \eta(G)$,

(b) $\lambda_2(G) \geq 2\eta(G)(1 - \cos\omega)$, and

(c) $\lambda_2(G) \geq 2(\cos\omega - \cos 2\omega)\eta(G) - 2\cos\omega(1-\cos\omega)\Delta(G)$.

It was discovered recently that graphs with large λ_2 (with respect to the maximal degree) have some properties which make them to be very useful objects in several applications. It is important that λ_2 imposes reasonably good bounds on several properties of graphs which are, for an explicit graph, very hard to compute. We shall mention three such applications. It should be noted that, in all of them, the graph invariants, on which λ_2 imposes non-trivial bounds, can be viewed as measures of connectivity.

Concentrators and expanders are graphs with certain high connectivity properties. They are used in the construction of switching networks that exhibit high connectivity, in the recent parallel sorting of Ajtai, Komlós, and Szemerédi [AKS], in the construction of linear-sized tolerant networks which arise in the study of fault tolerant linear arrays [AC], for the construction of the so-called superconcentrators which are extensively used in the theoretical computer science (e.g., the study of lower bounds in the algorithmic complexity (cf. [Va]), in the establishment of time space tradeoffs for computing various functions [Ab, JJ, To], the construction of graphs that are hard to pebble [LT, Pi, PTC], the construction of low complexity error-correcting codes, etc.), etc. Tanner [Ta] was probably the first who realized that the concentration and expanding properties of a graph can be analyzed by its (adjacency) eigenvalues. He observed that a small ratio of the subdominant adjacency eigenvalue to the dominant eigenvalue implies good expansion properties. Alon [A2] and Alon and Milman [AM1, AM2] followed Tanner's approach, but later they realized [A1, AM3, AGM] that the Laplacian spectrum of a graph (in particular the second smallest eigenvalue) appears more naturally in the study of expanding properties of graphs. [Ro] is an overview article about superconcentrators, and it includes also an exposition of some of the eigenvalue methods which we are trying to summarize here. In [AM3] the authors present several inequalities of the isoperimetric nature relating λ_2 and several other quantities in graphs. These results have analytic analogues [GM] in the theory of Riemannian manifolds where the role of λ_2 is played by the the smallest positive eigenvalue of the Laplacian differential operator on the Riemannian manifold (cf. also [Cha]).

The basic lemma of [AM3] is the following inequality. Let A and B be subsets of $V(G)$ at distance ρ (this is the minimal distance between a vertex in A and a vertex in

B), and let F be the set of edges which do not have both ends in A and do not have both ends in B. Then

$$|F| \geq \rho^2 \lambda_2(G) \frac{|A||B|}{|A|+|B|} \tag{6.3}$$

In particular, when $B = V \setminus A$, then $F = \delta A = \delta B$ (the *coboundary* of A, or of B) is the set of edges with one end in A and the other end outside A. In this case $\rho = 1$ and (6.3) implies

$$|\delta A| \geq \lambda_2(G) \frac{|A|(n-|A|)}{n} \tag{6.4}$$

A refinement of (6.3) is derived in [M3]. If A and B are subsets of $V(G)$ at distance $\rho > 1$ then

$$(\rho-1)^2 < \frac{\lambda_n(G)}{4\lambda_2(G)} \frac{(n-|A|-|B|)(|A|+|B|)}{|A||B|}. \tag{6.5}$$

The paper [AGM] considers the expansion properties of graphs and their applications. The main eigenvalue based lemma of [AGM] gives a lower bound on the number of neighbours of a set $X \subseteq V$. If $N(X)$ is the set of those neighbours of vertices of X which do not lie in X, then

$$|N(X)|^2 - 2(n-2|X|-\alpha n)|N(X)| - 4|X|(n-|X|) \geq 0 \tag{6.6}$$

where $\alpha = \frac{1}{2}(1+\frac{\Delta}{\lambda_2})$, and Δ is the maximum valency in G.

In [A1] expanders and graphs with large λ_2 are related. Expanders can be constructed from graphs which are c*-magnifiers* ($c \in \mathbb{R}^+$). These are graphs which are highly connected according to the following property. For every set X of vertices of G with $|X| \leq \frac{n}{2}$, the neighbourhood $N(X)$ of X contains at least $c|X|$ vertices. In [A1] it is shown that a graph G is $\frac{2\lambda_2}{\Delta+2\lambda_2}$ -magnifier and, conversely, if G is a c-magnifier then $\lambda_2(G) \geq \frac{c^2}{4+2c^2}$. The first result is based on (6.4), while the second one is a discrete version of the Cheeger inequality [Che] from the theory of Riemannian manifolds.

A strong improvement over the Alon's discrete version of the Cheeger inequality was obtained by the author [M2] in connection with another problem. The *isoperimetric number* $i(G)$ of a graph G is equal to

$$i(G) = \min\{\frac{|\delta X|}{|X|};\ X \subset V, 0 < |X| \leq \frac{|V|}{2}\}.$$

This graph invariant is very hard to compute, and even obtaining any lower bounds on $i(G)$ seems to be a difficult problem. It is shown in [M2] that

$$i(G) \geq \frac{\lambda_2(G)}{2} \tag{6.7}$$

and, moreover, a strong discrete version of the Cheeger inequality holds [M2]:

$$i(G) \leq \sqrt{\lambda_2(2\Delta - \lambda_2)} \tag{6.8}$$

where Δ is, as usual, the maximal degree in G. The reader is also referred to [M1].

We mention that these results are very important since they yield efficient checking procedures for several graph properties. For example, if $\lambda_2(G) = 2$ then we know by (6.7) that $i(G) \geq 1$. If, moreover, we find a cut X with $|\delta X| = |X|$ then we can conclude that $i(G) = 1$.

Besides the expansion properties and the isoperimetric numbers of graphs, an eigenvalue based inequality can be used for the max-cut problem [MP] (also the weighted case) which is known to be NP-hard. It is shown in [MP] that the number of edges MC(G) in a maximal cut in a graph G is bounded above by

$$MC(G) \leq \frac{n\lambda_n(G)}{4}. \tag{6.9}$$

Notice that $\lambda_n(G)$ is related to the second smallest eigenvalue of the complement of G (cf. Theorem 3.6).

The second eigenvalue is also related to some other graph invariants. One of the most interesting connections is its relation to the diameter and the mean distance of graphs. There is a lower bound

$$\mathrm{diam}(G) \geq \frac{4}{n\lambda_2(G)} \tag{6.10}$$

This bound was obtained by Brendan McKay [McK] but its proof appeared for the first time in [M3].

To get an upper bound one may use the inequality (6.5) which gives rise to an eigenvalue-based upper bound on the diameter of a graph [M3]:

$$\mathrm{diam}(G) \leq 2\left\lceil \sqrt{\frac{\lambda_n(G)}{\lambda_2(G)}}\sqrt{\frac{\alpha^2 - 1}{4\alpha}} + 1 \right\rceil \left\lceil \log_\alpha \frac{n}{2} \right\rceil \tag{6.11}$$

where α is any real number which is > 1. For any particular choice of n, λ_n, and λ_2 one can find the value of α which imposes the lowest upper bound on the diameter of the graph. See [M3] for details. A good general choice is $\alpha = 7$.

In [M3] another upper bound on the diameter of a graph is obtained

$$\operatorname{diam}(G) \le 2\left\lceil \frac{\Delta + \lambda_2(G)}{4\lambda_2(G)} \ln(n-1) \right\rceil. \tag{6.12}$$

This improves a bound of Alon and Milman [AM3]. It should be noted that Chung, Faber, and Manteuffel [CFM] found another bound:

$$\operatorname{diam}(G) \le \left\lceil \frac{\log(n-1)}{\log\big((\lambda_n + \lambda_2)/(\lambda_n - \lambda_2)\big)} \ln(n-1) \right\rceil.$$

In [M3], some bounds on the mean distance $\bar\rho(G)$ are derived. Recall that the mean distance is equal to the average of all distances between distinct vertices of the graph. A lower bound is

$$(n-1)\bar\rho(G) \ge \frac{2}{\lambda_2(G)} + \frac{n-2}{2} \tag{6.13}$$

and an upper bound, similar to (6.12), is

$$\bar\rho(G) \le \frac{n}{n-1}\left\lceil \frac{\Delta + \lambda_2(G)}{4\lambda_2(G)} \ln(n-1) \right\rceil. \tag{6.14}$$

There is also an upper bound on $\bar\rho(G)$ related to the inequality (6.11). Cf. [M3].

Some inequalities relating graph invariants to the spectrum of the adjacency matrix of a graph can as well be formulated in terms of the Laplacian spectrum — usually obtaining even stronger results this way. As an example we extend a Hoffman–Lovász' bound [CDS, Lo] on the *independence number* $\alpha(G)$ of a graph. They proved that a d-regular graph G has $\alpha(G) \le n(1 - d/\lambda_n)$.

Let G be a graph of order n with vertices of degrees $d_1 \le d_2 \le \cdots \le d_n$. Set

$$e_r = \frac{1}{r}(d_1 + d_2 + \cdots + d_r)\ , \qquad 1 \le r \le n.$$

Assume we have an independent set R of vertices of size r. Define a vector $x \in \ell^2(V(G))$ by setting

$$x_v = \begin{cases} 0, & v \in R \\ 1, & v \notin R \end{cases}$$

By (6.2′),

$$\lambda_n(G) \sum_{u \in V} \sum_{v \in V} (x_u - x_v)^2 \geq 2n \sum_{uv \in E} (x_u - x_v)^2$$

which reduces to $\lambda_n r(n-r) \geq n|\delta R| \geq nre_r$. It follows that

$$r \leq \frac{n(\lambda_n - e_r)}{\lambda_n} \tag{6.15}$$

6.3. Theorem. If r_0 is the smallest number r for which (6.15) fails then

$$\alpha(G) \leq r_0 - 1. \tag{6.16}$$

It is interesting that large graphs of bounded genus and with bounded maximal degree have small λ_2 .

6.4. Theorem. Let G be a graph of order n , with maximal vertex degree Δ and genus g . If $n > 18(g+2)^2$ then

$$\lambda_2(G) \leq \frac{6(g+2)\Delta}{\sqrt{n/2} - 3(g+2)}.$$

Proof. Boshier [Bo] proved that under the hypothesis of the theorem

$$i(G) \leq \frac{3(g+2)\Delta}{\sqrt{\frac{n}{2}} - 3(g+2)}$$

where $i(G)$ is the isoperimetric number of G . The inequality (6.7) now completes the proof.

It would be interesting to have a "direct" proof of Theorem 6.4. We believe that such a proof would yield even better inequality, between λ_2 and the genus of a graph, than outlined above.

C. Maas [Ma] studied extensively how can $\lambda_2(G)$ change if we delete or insert an edge into G . He derived several upper and lower bounds on this change, some of them being quite non-obvious. In [Ma] there is also a result which was obtained independently by R. Merris [Me2]. See also [F4].

6.5. Theorem. For a tree T , $\lambda_2(T) \leq 1$, with equality if and only if T is a star.

Three interesting notions are introduced in [Ma], depending on λ_2 and the corresponding eigenspace: *permeability* of a graph, the *well-connectedness* of pairs of vertices, and a measure to relate how *good position* have particular vertices. It is shown on some examples that the notions introduced behave in correspondence with our intuitive notion of permeability, well connected pairs of vertices, and a good (strategic, central) position in a network. Merris [Me2] also found that a kind of a central position in a tree can be defined by using λ_2 and the corresponding eigenvectors.

Let us finish this section with few words about infinite graphs. Let G be a locally finite countable graph with bounded vertex degrees. Its Laplacian matrix $Q(G)$ gives rise to a self-adjoint linear operator on the Hilbert space $\ell^2(V)$. Its spectrum $\sigma(G)$ is called the Laplacian spectrum of G. It is worth mentioning that the role of λ_2 is replaced by $\lambda = \inf \sigma(G)$. It might happen that $\lambda = 0$ for a connected graph G. Indeed, this is true for any graph of polynomial growth. More details can be found in [BMS, M1, MW], especially about the relation between λ, the growth, and the isoperimetric number of G.

7. CHARACTERISTIC VALUATIONS

An eigenvector of $\lambda_2(G)$ is called a *characteristic valuation* of G. The characteristic valuations, especially their sign structure, have been studied by Fiedler [F2], and Merris and Grone [Me2, GM1, GM2]. We shall collect here only the most interesting results of these papers.

7.1. Theorem. [F2,F4] Let G be a connected weighted graph with non-negative weights, and $y = (y_v)_{v \in V(G)}$ a characteristic valuation of G. For $r \geq 0$ let

$$S(r) = \{v \in V(G) \,|\, y_v \geq -r\}.$$

Then the subgraph induced on $S(r)$ is connected.

A similar result holds for $r \leq 0$ and $S'(r) = \{v \,|\, y_v \leq -r\}$. It is an interesting corollary to Theorem 7.1 that if $c \geq 0$ is such a constant that $y_v \neq c$ for all vertices v of

G, and $S_1 = \{v \mid y_v > c\}, S_2 = V(G) \setminus S_1$, then the subgraphs of G induced on S_1 and S_2 are both connected.

7.2. Theorem. [F2] Let G be a connected graph, $y = (y_v)_{v \in V(G)}$ a characteristic valuation of G, and v a cut-vertex of G. Denote by $G_1, G_2, \ldots, G_r$ the components of $G - v$. Then:

(a) If $y_v > 0$ then exactly one G_i contains a vertex u with $y_u < 0$. All vertices in other components G_j have positive y-value.

(b) If $y_v = 0$ and some G_i contains positively and negatively valuated vertices, then all the remaining components are 0-valuated.

7.3. Theorem. [F2] Let G be a connected graph with a characteristic valuation y. Two possibilities arise:

(a) There exists a unique block B_0 of G with both, positive and negative y-values. All other blocks have either all positive, or all negative, or only zero values.

(b) No block of G contains positive and negative values simultaneously. In this case there is a **unique** cut-vertex v with $y_v = 0$ which has a neighbour u with $y_u \neq 0$.

In the case when G is a tree, the above results are strengthened in [F2] and discussed in greater details in [Me2, GM1, GM2]. In [GM1] the *trees of type I* are investigated. These are trees with a characteristic valuation y such that $y_v = 0$ for some vertex v of the tree. It is shown that every tree T of type I contains a unique vertex w such that $y_w = 0$ for every characteristic valuation y of T. This vertex is called a *characteristic vertex* of T. *Branches,* i.e. the components of $T - w$ are characterized as *active* or *passive* (every characteristic valuation is 0 on a passive branch). Their properties with respect to $\lambda_2(T)$ are investigated. In [GM2] the authors consider a more general family of matrices, $Q^{\alpha,\beta} = \alpha D(G) + \beta A(G)$ ($\alpha, \beta \in \mathbb{R}$).

Characteristic valuations can be efficiently used to obtain well-behaved heuristic algorithms for various problems. Let y be a characteristic valuation of G and let $A = \{v \in V(G) | y_v \geq 0\}$, $B = V \backslash A$. It follows from the proof of Theorem 4.2 in [M2] that the partition $V = A \cup B$ is not too far from an optimal partition $V = A^\circ \cup B^\circ$ where the optimum means that A° and B° have minimal possible average outdegree. This fact can be applied to devise several *divide-and-conquer* algorithms: One solves a problem separately on A and on B and then tries to combine solutions to get an acceptable solution for the graph G.

Another type of problems where characteristic valuations can be used are *optimal labeling problems*, e.g., the bandwidth, or the min-sum problem. It is requested to arrange the vertices of a graph in a linear order $v_1, v_2, \cdots, v_n$ in such a way that the edges will not do too long jumps (if $v_i v_j$ is an edge then $|i-j|$ should be small). A reasonably good ordering is obtained by ordering the vertices of G with respect to the values of a characteristic valuation y, i.e., $v \le u$ if $y_v \le y_u$. The eigenvalue $\lambda_2(G)$ also gives a lower bound on the average square of jumps for *any* linear ordering $v_1, \cdots, v_n$ of $V(G)$. If $e = v_i v_j$ then $jump(e) := |i-j|$. Then

$$\sum_{e \in E(G)} [jump(e)]^2 \ge \lambda_2(G) \frac{n(n^2-1)}{12}. \qquad (7.1)$$

The details about (7.1) with many different extensions will appear elsewhere [JM].

8. MISCELLANEOUS

In case of regular graphs, all results about the adjacency spectrum of graphs carry over to results about the Laplacian spectrum, since for a d-regular graph G

$$\mu(G,x) = (-1)^n \varphi(G, d-x) \tag{8.1}$$

where φ is the characteristic polynomial of $A(G)$. But even in the general, non-regular case, the Laplacian spectrum of G is related to the adjacency spectrum of some graph G'. Let Δ be the maximal valency of G, and let G' be the graph obtained from G by adding, at each vertex $v \in V(G) = V(G')$, $\Delta - d(v)$ loops. Thus G' is Δ-regular and $Q(G) = Q(G')$. Consequently,

$$\mu(G,x) = \mu(G',x) = (-1)^n \varphi(G', \Delta - x). \tag{8.2}$$

D.L. Powers has assembled a catalogue containing the eigenvalues and eigenvectors of the adjacency and the Laplacian matrices of all connected graphs with up to 6 vertices [P2] and all trees with up to 9 vertices [P1].

Kel'mans [K3] found a class of graphs which is characterized by the Laplacian spectrum. In general there are many cospectral non-isomorphic graphs. For example, it can be shown that almost all trees are cospectral.

R. Merris [Me2] derived some inequalities between the coefficients of the Laplacian polynomial $\mu(G,x)$ and the coefficients of the chromatic polynomial of G (G is a connected simple graph).

Let G be a simple graph. For a vertex $v \in V(G)$, let the *star degree* of v be defined as

$$\operatorname{stardeg}(v) = \begin{cases} 0, & \text{if no neighbour of } v \text{ is a pendant vertex} \\ k-1, & \text{if } v \text{ has } k \geq 1 \text{ pendant neighbours} \end{cases}.$$

The *star degree* of the graph G is then equal to the sum of star degrees of all its vertices. I. Faria [Fa] proved that the star degree of G is equal to the multiplicity of $x = 1$ as the root of the permanental polynomial $\operatorname{per}(xI - B(G))$, $B(G) = D(G) + A(G)$. If G is bipartite then the permanental polynomial of $B(G)$ is equal to the permanental polynomial of the Laplacian matrix $Q(G)$. The author mentions (without an explicit proof) that in the case of characteristic polynomials of $B(G)$ and $Q(G)$, we can only conclude that the star degree of G is at most equal to the multiplicity of $x = 1$ as the zero of these polynomials. Some other authors studied the permanental polynomial of $Q(G)$ [BG, Me1].

C.D. Godsil [Go] proved that the polynomial $\psi(G,S;x) = \sum f_k x^k$, where $S \subseteq E(G)$ and f_k is the number of spanning trees of G with exactly k edges in S, has only real zeros. A corresponding result holds for a generalization of $\psi(G,S;x)$ to unimodular matroids and numbers of bases with specified number of elements in given subsets of the matroid. Is there a corresponding generalization of $\mu(G,x)$ to matroids where the coefficients of the polynomial relate to bases of the matroid in the same way as the coefficients of $\mu(G,x)$ relate to spanning trees of G (cf. Theorem 4.3)?

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