SPECTRAL GRAPH THEORY: SOME ELEMENTARY BUT IMPORTANT RESULTS[1]

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Abstract. *I have presented several simple results of mine related to graph spectra which in turn appeared to be of some importance in the development of spectral graph theory. Results relevant to Chemistry are included as well.*

1 Introduction

Spectral graph theory is a mathematical theory in which linear algebra and graph theory meet. For any graph matrix M we can build a spectral graph theory in which graphs are studied by means of eigenvalues of the matrix M. This theory is called *M-theory.* In order to avoid confusion, to any notion in this theory a prefix M- could be added (e.g., M-eigenvalues). Frequently used graph matrices are the adjacency matrix A, the Laplacian $L = D - A$ and the signless Laplacian $Q = D + A$, where D is a diagonal matrix of vertex degrees. *The* spectral graph theory includes all particular theories together with interaction tools.

Originally, A-theory was developed. The Q-theory has been established in last several years.

The adjacency matrix A of a graph G, with n vertices, is the matrix whose element a_{ij} is equal to the number of the edges, which lead from the vertex i to the vertex j. The spectrum of the graph G is the set of solutions λ_i $(1 = 1, \ldots, n)$ of the characteristic equation $\det(\lambda I - A) = 0$ of the matrix A, i. e. the family of eigenvalues of A.

We use standard notation K_n, C_n and P_n for the complete graph, cycle and the path on n vertices and K_{n_1,n_2} for the bicomplete graph on $n_1 + n_2$ vertices.

I was in position to take part in founding A-theory and Q-theory and was forced to describe some basic results. Any educated mathematician would do approximately the same in my position!

In general, I tend to simplify the things if possible, contrary to some researchers who want to make everything complicate. The simplicity, in my opinion, is not a weakness of a theory provided the theory is good.

My results include Theorems 2, 3, 4, 5, 6, 8, 9, 11, 12, 13 and 15 - 19, Definitions 1, 2, 5 and 7, constructions of some cospectral graphs (Section 4) and related formulas as described in Sections 3 - 10. A special contribution was to show that the Hückel molecular orbital

[1] Recently W. So and W. Haemers asked who was first to observe that bipartite graphs are characterized by their spectra (Theorem 3 below). That inspired me to prepare this paper.

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theory from Chemistry and the theory of graph spectra are essentially the same, as described in Section 9. Most of these results appeared in my thesis [13] or/and in the monograph [18].

2 Thesis and the monograph

In my thesis [13], defended on May 27, 1971, I wrote:

> While writing this paper, I have aimed at the following goals: 1. To supplement the existing procedures of the spectral method by original contributions; 2. To connect the results of various authors; 3. To show by concrete examples the possibilities of application of the spectral method; 4. To expose in one place all the important results of this discipline from a unique outlook.

The formal supervisor was D.S. Mitrinović but the thesis was accepted on the basis of informal reports by L. Collatz and H. Sachs.

The thesis, originally prepared in Serbian, has been published in English in a condensed form [13]. It attracted attention of American mathematician Richard Bellman who sent me the following letter on July 29, 1972:

> Dear Dr. Cvetković, I noted with great interest your paper "Graphs and Their Spectra". Have you given any thought to extending these results and collecting them in book form? If so, I would be glad to consider it for my Academic Press series.

H. Sachs even earlier suggested to write a monograph with Deutscher Verlag der Wissenschaften.

This led after some time to publication of the book [18]. The book has been widely used and cited a few thousand times in the literature.

3 Basic properties of graph spectra

I realized that the well established Perron-Frobenius theory of non-negative matrices is relevant for the theory of graph spectra. In the thesis [13] and in the monograph [18] I have collected all useful theorems from the Perron-Frobenius theory and classified basic implications of them.

Spectral properties of irreducible non-negative matrices are described by the following theorem of *Frobenius* and this has several immediate corollaries.

Theorem 1. *An irreducible non-negative matrix A always has a positive eigenvalue r that is a simple root of the characteristic polynomial. The modulus of any other eigenvalue does not exceed r. To the "maximal" eigenvalue r there corresponds a positive eigenvector. Moreover, if A has h eigenvalues of modulus r, then these numbers are all distinct and are roots of the equation $\lambda^h - r^h = 0$. More generally: the whole spectrum $[\lambda_1 = r, \lambda_2, \ldots, \lambda_n]$ of A, regarded as a system of points in the complex λ-plane, is mapped onto itself under a rotation of the*

plane by the angle $\frac{2\pi}{h}$. *If* $h>1$, *then by a permutation of rows and the same permutation of columns* A *can be put into the following "cyclic" form*

$$A = \begin{Vmatrix} O & A_{12} & O & \dots & O \\ O & O & A_{12} & \dots & O \\ \vdots & & & \ddots & \\ O & O & O & \dots & A_{h-1,h} \\ A_{h1} & O & O & \dots & O \end{Vmatrix},$$

where there are square blocks along the main diagonal.

The adjacency matrix of an undirected multigraph G is symmetric (and, therefore, Hermitian) and the spectrum of G, containing only real numbers, according to Theorem 1 lies in the segment $[-r, r]$. The largest eigenvalue r is also called the *index* of G.

For the smallest eigenvalue q of the spectrum of a graph G the inequality $-r \le q \le 0$ holds. For the graph without edges we have $q = 0$. Otherwise $q \le -1$.

According to the foregoing, the following theorem describes the fundamental spectral properties of (undirected) graphs [13], [18].

Theorem 2. *For the spectrum* $[\lambda_1, \lambda_2, \dots, \lambda_n]$ *of an (undirected) graph* G *the following statements holds*:

1° *The numbers* $\lambda_1, \lambda_2, \dots, \lambda_n$ *are real and* $\lambda_1 + \lambda_2 + \dots + \lambda_n = 0$.

2° *If* G *contains no edges, we have* $\lambda_1 = \dots = \lambda_n = 0$.

3° *If* G *contains at least one edge, we have*

$$1 \le r \le n - 1\,, \tag{1}$$

$$-r \le q \le -1\,. \tag{2}$$

In (1) *the upper bound is attained if and only if* G *is a complete graph, while the lower bound is reached if and only if the components of* G *consist of graphs* K_2 *and possibly* K_1. *In* (2) *the upper bound is reached if and only if the components of* G *are complete graphs, and the lower bound if and only if a component of* G *having the greatest index is a bipartite graph. If* G *is connected, the lower bound in* (1) *is replaced by* $2\cos\frac{\pi}{n+1}$. *Then equality holds if and only if* G *is a path.*

The following theorem appeared in [13] as Theorem 4.10.

Theorem 3. *A graph* G *is regular (of degree* λ_1*) if and only if*

$$n\lambda_1 = \lambda_1^2 + \lambda_2^2 + \dots + \lambda_n^2.$$

If equality holds, the number of components of G *is equal to the multiplicity of the eigenvalue* λ_1.

Thus regularity (together with the connectedness property) can be recognized from the spectrum.

The proof is based on the properties of the Rayleigh quotient. The theorem is implicitly contained in [4] and [12].

Theorem 3 is very useful in many existing characterizations of regular graphs by their spectra starting from characterizations of the cubic lattice graph [12]. Many examples can be found in [24].

Next we turn to the bipartiteness of graphs.

It is proved in [4] that a bipartite graph has a symmetric spectrum. This fact was known even earlier in chemical literature under the name the *Pairing Theorem* [7], [5]. In [8] a new proof of this theorem and the proof of the inverse theorem are given:

Theorem 4.[3] *Connected, finite, undirected graph, without loops and with at least two vertices, is bipartite if and only if, its spectrum, considered as a set of points on the number axis, is symmetric with respect to the point zero.*

This characterization of bipartite graphs appeared for the first time in my paper [8]. The theorem appears also in my book "Spectra of Graphs" as Theorem 3.11 on. p. 87, where other related references can be found. The paper [8] appears in the book as reference [Cve1].

The proof in [8] uses the Frobenius theorem (Theorem 1) what nowadays can be considered as shooting with cannons on small birds. In recent book [24] the proof uses the fact that in the case of a symmetric spectrum all the odd spectral moments are zero and the graph has no cycles of odd length.

Actually, from the proof in [8] it is clear that only bipartite graphs, from the considered class of graphs, have in the spectrum the number $-r$, where, r is the largest number from the spectrum.

Hence, for connected graphs we have a substantially stronger result:

Theorem 5. *A connected graph G is bipartite if and only if $\lambda_1 = -\lambda_n$.*

This important characterization of connected bipartite graphs is proved in [13] (Theorem 4.3) using the Frobenius theorem. Again this can be done with simpler tools (see [24], Theorem 3.2.4). See Section 8 for an application of Theorem 5.

4 Cospectral graphs

The term "a pair of isospectral non-isomorphic graphs" was denoted in [13] as a PING. Nowadays we use the term "cospectral" instead of "isospectral".

The smallest PING was found in [13]. It consists of graphs $C_4 \cup K_1$ and $K_{1,4}$.

This example was generalized in the same paper. The graph, having as components s isolated vertices and one bicomplete graph K_{n_1,n_2} has the spectrum containing numbers $\sqrt{n_1 n_2}, -\sqrt{n_1 n_2}$ and $n_1 + n_2 - 2 + s$ numbers equal to 0. Consider the graph with the spectrum: $\sqrt{m}, -\sqrt{m}$ and $n-2$ numbers equal to 0 (m a natural number). This spectrum may belong to each of graphs of the above described type whose parameters n_1, n_2, s satisfy

[3] The theorem is formulated in [24] in a more condensed form: *A graph G is bipartite if and only if its spectrum is symmetric with respect to the origin.*

the equations $n_1 + n_2 - 2 + s = n,\ n_1 n_2 = m$. These equations can have obviously several solutions in the set of natural numbers (s can be equal to 0).

The spectral structure of graphs having the largest eigenvalue not greater than 2 was completely described in [20]. This includes a construction of all cospectral graphs in the considered class of graphs.

First examples of cubic cospectral graphs have been found in [2], [3]. There are three pairs of cospectral cubic graphs on 14 vertices.

5 Refinements using eigenvectors and graph angles

A graph is completely determined by eigenvalues and eigenvectors in the following sense. Let A be the adjacency matrix of a graph G with vertices $1, 2, \ldots, n$ and eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. If $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$ are linearly independent eigenvectors of A corresponding to $\lambda_1, \lambda_2, \ldots, \lambda_n$ respectively, if $V = (\mathbf{v}_1|\mathbf{v}_2|\cdots|\mathbf{v}_n)$ and if $D = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, then

$$A = VDV^{-1}.$$

Since G is determined by A, we have proved, [18], p. 44,

Theorem 6. *Any graph is determined by its eigenvalues and a basis of corresponding eigenvectors.*

We may construct an orthonormal basis of eigenvectors $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n$ by stringing together orthonormal bases of eigenspaces. If $U = (\mathbf{u}_1|\mathbf{u}_2|\cdots|\mathbf{u}_n)$ then $U^{-1} = U^T$ and we have

$$A = UDU^T, \tag{3}$$

a relation which we exploit in the next section.

Since eigenvectors are not graph invariants it is reasonable to extend eigenvalue based techniques by some invariants of the eigenspaces called *graph angles*.

Let G be a graph on n vertices with distinct eigenvalues $\mu_1, \mu_2, \ldots, \mu_m$ ($\mu_1 > \mu_2 > \cdots > \mu_m$) and let $S_1, S_2, \ldots, S_m$ be the corresponding eigenspaces. Let $\{e_1, e_2, \ldots, e_n\}$ be the standard (orthonormal) basis of $\mathbf{R}^n$.

Definition 1. *The numbers $\alpha_{pq} = \cos\beta_{pq} (p = 1, 2, \ldots, m; q = 1, 2, \ldots, n)$, where β_{pq} is the angle between S_p and e_q, are called graph angles. The sequence α_{pq} $(q = 1, 2, \ldots, n)$ is called the eigenvalue angle sequence corresponding to the eigenvalue μ_p $(p = 1, 2, \ldots, m)$. We also define the angle matrix of G, i.e. an $m \times n$ matrix (m is the number of its distinct eigenvalues, while n is the order of G) as a matrix (α_{ij}). This matrix is a graph invariant if its columns are ordered lexicographically. The rows of the angle matrix are called the standard eigenvalue angle sequences.*

Let $x_i = (x_{i1}, x_{i2}, \ldots, x_{in})$ $(i = 1, 2, \ldots, n)$ be orthonormal eigenvectors of G. Define $M_p = \{j \mid Ax_j = \mu_p x_j\}$. We have $\alpha_{pq}^2 = \sum_{j \in M_p} x_{jq}^2$ for squares of angles of G. This formula holds for any choice of orthonormal eigenvectors of G (cf. [22], p. 76).

Definition 2. *The cosines $\beta_1, \beta_2, \ldots, \beta_m$ of angles between the vector $(1, 1, \ldots, 1) \in \mathbf{R}^n$ and eigenspaces $S_1, S_2, \ldots, S_m$ are called main angles of the graph. An eigenvalue is called main if the corresponding main angle is different from 0. The set of main eigenvalues is called the main part of the spectrum.*

The main part of the spectrum has been introduced in [10].

An overview of results on graph angles is given in [22] including the characterizing properties of graph angles. A survey on main angles appeared in [36].

Let G be a graph with adjacency matrix A, and let $N_k(j) = a_{jj}^{(k)}$, the number of walks of length k in G originating and terminating at vertex j (see Theorem 7). Let $\mathcal{H}_j(t)$ be the generating function $\sum_{k=0}^{\infty} N_k(j)t^k$. We can obtain [22], p. 82,

$$N_s(j) = a_{jj}^{(s)} = \sum_{i=1}^{n} \mu_i^s \alpha_{ij}^2,$$

$$\mathcal{H}_j(t) = \sum_{k=0}^{\infty} t^k \sum_{i=1}^{m} \alpha_{ij}^2 \mu_i^k = \sum_{i=1}^{m} \frac{\alpha_{ij}^2}{1 - \mu_i t}.$$

On the other hand, we have $\mathcal{H}_j(t) = 1 + d_j t^2 + 2t_j t^3 + \cdots$, where d_j is the degree of vertex j and t_j is the number of triangles containing j.

The degree d_j of the vertex j, and the number t_j of triangles containing the vertex j, are given by

$$d_j = \sum_{i=1}^{m} \alpha_{ij}^2 \mu_i^2, \qquad t_j = \frac{1}{2} \sum_{i=1}^{m} \alpha_{ij}^2 \mu_i^3.$$

The following formulas are also useful.

Let $P_G(\lambda) = \det(\lambda I - A)$ be the characteristic polynomial of the graph G. The generating function can be obtained by the formula

$$\mathcal{H}_j^G(t) = P_{G-j}(\frac{1}{t})/tP_G(\frac{1}{t}),$$

since

$$P_{G-j}(x) = P_G(x) \sum_{i=1}^{m} \frac{\alpha_{ij}^2}{x - \mu_i}.$$

6 Counting walks

We can use eigenvalues and eigenvectors to count walks in a graph.

Definition 3. *By a walk of length k in a graph (or digraph) we mean any sequence of (not necessarily different) vertices $x_1, x_2, \ldots, x_k, x_{k+1}$ such that for each $i = 1, 2, \ldots, k$ there is an edge (or arc) from x_i to x_{i+1}. The walk is closed if $x_{k+1} = x_1$.*

Counting walks with specified properties in a graph (or digraph) is related to graph spectra by the following well-known result.

Theorem 7. *If A is the adjacency matrix of a graph, then the (i,j)-entry $a_{ij}^{(k)}$ of the matrix A^k is equal to the number of walks of length k that originate at vertex i and terminate at vertex j.*

Thus, for example, the number of closed walks of length k is equal to the k-th spectral moment, since $\sum_{i=1}^{n} a_{ii}^{(k)} = \mathrm{tr}(A^k) = \sum_{i=1}^{n} \lambda_i^k$.

Many combinatorial enumeration problems can be reduced to the enumeration of walks in a suitably chosen graph or digraph. Also, formulas giving the number of walks in terms of eigenvalues and eigenvectors represent a link between spectral and structural properties of a graph, and this is a very useful auxiliary tool in treating many problems on graphs. An important notion related to the number of walks is the main part of the spectrum, described in Section 5.

Let G denote a graph with adjacency matrix A and let $U = (u_{ij})$, an orthogonal matrix of eigenvectors of A as described in Section 5. Then, according to (3),

$$a_{ij}^{(k)} = \sum_{s=1}^{n} u_{is} u_{js} \lambda_s^k. \tag{4}$$

The number N_k of all walks of length k in G is given by

$$N_k = \sum_{i,j} a_{ij}^{(k)} = \sum_{s=1}^{n} \left(\sum_{i=1}^{n} u_{is} \right)^2 \lambda_s^k.$$

Thus we have proved

Theorem 8. *The total number N_k of walks of length k in a graph G is given by*

$$N_k = \sum_{s=1}^{n} C_s \lambda_s^k \quad (k = 0, 1, 2, \ldots),$$

where $C_s = \left(\sum_{i=1}^{n} u_{is}\right)^2$.

I proved this theorem in a slightly different form in [10]. When preparing the book [18] I found the theorem in this form and it appeared in [18] as Theorem 1.8 on p. 44. Another proof of the theorem appears in [34].

The formula of Theorem 8 can be rewritten in the form

$$N_k = \sum_{s=1}^{m} D_s \mu_s^k \quad (k = 0, 1, 2, \ldots), \tag{5}$$

where $\mu_1, \mu_2, \ldots, \mu_m$ are distinct eigenvalues.

Note that the quantities D_s are related to main angles β_s, i.e. $D_s = n\beta_s^2$ $(s = 1, 2, \ldots, m)$. Given the eigenvalues of G, knowledge of the main angles of G is equivalent to knowledge of the *walk generating function*

$$W_G(t) = \sum_{k=0}^{\infty} N_k t^k,$$

where N_k is the number of walks of length k in G. For by formula (5) we have

$$W_G(t) = n \sum_{p=1}^{m} \beta_p^2/(1 - t\mu_p).$$

The walk generating function can be expressed also in terms of characteristic polynomials of the graph and of its complement [10]:

$$W_G(t) = \frac{1}{t} \left\{ (-1)^n \frac{P_{\overline{G}}\left(-\frac{t+1}{t}\right)}{P_G\left(\frac{1}{t}\right)} - 1 \right\}.$$

Main angles are relevant also for the theory of graph divisors.

Definition 4. *Given an $s \times s$ matrix $B = (b_{ij})$, let the vertex set of a graph G be partitioned into (non-empty) subsets $X_1, X_2, \ldots, X_s$ so that for any $i, j = 1, 2, \ldots, s$ each vertex from X_i is adjacent to exactly b_{ij} vertices of X_j. The multidigraph H with adjacency matrix B is called a front divisor of G, or briefly, a divisor of G.*

The concept of a divisor of a graph was introduced by H. Sachs [38], [39]. The existence of a divisor means that the graph has a certain structure; indeed, a divisor can be interpreted as a homomorphic image of the graph. On the other hand, by Theorem 2.4.3 of [22], the characteristic polynomial of a divisor divides the characteristic polynomial of the graph (i.e. the spectrum of a divisor is contained in the spectrum of the graph). In this way the notion of a divisor can be seen as a link between spectral and structural properties of a graph [30]. Divisors have been considered in [34] under the name *equitable partitions*.

The role of main eigenvalues in the theory of graph divisors is explained by the next theorem from [15].

Theorem 9. *The spectrum of any divisor H of a graph G includes the main part of the spectrum of G.*

Since the largest eigenvalue r of a graph always belongs to the main part of the spectrum we have the following result.

Corollary. [15] *Any divisor of a graph G has the index of G as an eigenvalue.*

It was conjectured in [34] that the spectrum of a divisor H with the smallest number of vertices is just the main part of the spectrum of G. Theorem 9 confirms one of the two inclusions implicit in this conjecture. The reverse inclusion does not hold in general, as shown by a counterexample in [15].

7 Interlacing theorem

The so called Interlacing Theorem (Theorem 10) plays an important role in spectral graph theory and its applications.

Recall that the matrix A with complex entries a_{ij} is called *Hermitian* if $A^T = \overline{A}$, i.e. $a_{ji} = \overline{a}_{ij}$ for all i, j.

Theorem 10. (see, e.g., [18], p. 19) Let A be a Hermitian matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and let B be one of its principal submatrices. If the eigenvalues of B are $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_m$ then $\lambda_{n-m+1} \leq \mu_i \leq \lambda_i$ $(i = 1, \ldots, m)$

The inequalities of this theorem are known as *Cauchy's inequalities* and the whole theorem is known as the *Interlacing Theorem.*

Usually, A is the adjacency matrix of a graph G and B is the adjacency matrix of an induced subgraph H of the graph G.

On the basis of the spectrum the inequalities for the number of internal stability $\alpha(G)$ and the number $k(G)$ of vertices of the maximal complete subgraph of the graph G can easily be obtained using Theorem 10. It seems that I was the first to use the Interlacing Theorem in the theory of graph spectra. An obvious idea how to apply this theorem led to the following result [13], [14].

Theorem 11. *The number of internal stability $\alpha(G)$ of the graph G satisfies the inequality $\alpha(G) \leq p_0 + min(p_-, p_+)$, where p_-, p_0, p_+ denote the numbers of eigenvalues, smaller, equal and greater than zero in the spectrum of G.*

In [14] an inequality for the size of a maximal clique and for the chromatic number of a graph are obtained as well.

Theorem 11 has been cited very much in the literature, among other places in books [31] and [1]. It is said on p. 216 of [31] that this theorem "seems surprisingly useful".

8 Application of the spectral method

The main idea of spectral graph theory is to use graph eigenvalues to prove statements on graphs which do not involve eigenvalues. I shall describe two such contributions of mine.

1. The set of vertices of the product $G_1 \times G_2$ of graphs G_1, G_2 is the Cartesian product of the sets of vertices of the graphs G_1, G_2. If x_i and y_i are vertices of the graph G_i $(i = 1, 2)$ the vertices $(x_1, , x_2)$ and (y_1, y_2) of $G_1 \times G_2$ are adjacent if, and only if, x_1, y_1 are adjacent in G_1 and x_2, y_2 are adjacent in G_2.

It is proved in [41] that the product of two finite, connected graphs is a connected graph if, and only if, at least one of the graph - factors has an odd cycle. In 1969 I proved this theorem using graph eigenvalues in the following way.

Let r_1 and q_1 be the largest and the least eigenvalue of G_1 and r_2 and q_2 the same quantities for G_2. Since eigenvalues of $G_1 \times G_2$ are all possible products of an eigenvalue of G_1 and of an eigenvalue of G_2, the largest eigenvalue of $G_1 \times G_2$ is $r_1 r_2$. By the Perron-Frobenius theory of non-negative matrices this eigenvalue is simple with a positive eigenvector unless $q_1 = -r_1$ and $q_2 = -r_2$ in which case $r_1 r_2$ is a twofold eigenvalue. In the first case $G_1 \times G_2$

is connected. By Theorem 5 the second case appears if and only if both graphs G_1, G_2 are bipartite and $G_1 \times G_2$ appears to be disconnected.

I published this result in a more general setting in [9].

We shall define the p-sum ($p = 1, \ldots, n$) of graphs $G_1, \ldots, G_n$. The set of vertices of the p-sum is the Cartesian product of the sets of vertices of the graphs $G_1, \ldots, G_n$. If x_i and y_i are vertices of the graph G_i ($i = 1, \ldots, n$) the vertices of the p-sum $(x_1, \ldots, x_n)$ and $(y_1, \ldots, y_n)$ are adjacent if, and only if, exactly p of n pairs (x_i, y_i) $(i = 1, \ldots, n)$ are the pairs of the adjacent vertices in corresponding graphs and if for the other $n - p$ pairs holds $x_i = y_i$). If $p = n$, the p-sum is called the product of graphs and in the case $p = 1$ - the sum of graphs.

The eigenvalues of the p-sum are elementary symmetric functions of order p of eigenvalues of graphs $G_1, \ldots, G_n$. Similar reasoning as above leads to the following theorem.

Theorem 12. *Let $G_1, \ldots, G_n$ be finite, connected, undirected graphs, without loops and multiple edges and with at least two vertices. p-sum of these graphs is a connected graph if, and only if, one of the following conditions holds: 1. p is equal to n and at most one of the graphs $G_1, \ldots, G_n$ is bipartite, 2. p is odd and less than n, 3. p is even and less than n, where at least one of the graphs $G_1, \ldots, G_n$ is not bipartite.*

If p is equal to n and exactly $l(> 1)$ of the graphs $G_1, \ldots, G_n$ are bipartite, the p-sum has 2^{l-1} components. If p is even and less than n and all the graphs $G_1, \ldots, G_n$ are bipartite, the p-sum has two components.

By the above facts, the following theorem from [9] can also be easily proved using Theorem 5.

Theorem 13. *The p-sum from Theorem 12 is a bipartite graph if, and only if, one of the following conditions holds: 1. p is equal to n and at least one of the graphs $G_1, \ldots, G_n$ is bipartite, 2. p is odd and less than n and all the graphs $G_1, \ldots, G_n$ are bipartite.*

Theorems 12 and 13 have been generalized in [13] to a very general graph operation called NEPS (*non-complete extended p-sum*) of graphs.

Definition 5. *Let $\mathcal{B}$ be a set of non-zero binary n-tuples, i.e. $\mathcal{B} \subseteq \{0,1\}^n \backslash \{(0, \ldots, 0)\}$. The NEPS of graphs $G_1, \ldots, G_n$ with basis $\mathcal{B}$ is the graph with vertex set $V(G_1) \times \cdots \times V(G_n)$, in which two vertices, say $(x_1, \ldots, x_n)$ and $(y_1, \ldots, y_n)$, are adjacent if and only if there exists an n-tuple $\beta = (\beta_1, \ldots, \beta_n) \in \mathcal{B}$ such that $x_i = y_i$ whenever $\beta_i = 0$, and x_i is adjacent to y_i (in G_i) whenever $\beta_i = 1$.*

Clearly the NEPS construction generates many binary graph operations in which the vertex set of the resulting graph is the Cartesian product of the vertex sets of the graphs on which the operation is performed. We mention some special cases in which a graph is the NEPS of graphs $G_1, \ldots, G_n$ with basis $\mathcal{B}$. In particular, for $n = 2$ we have the following familiar operations:

(i) the *sum* $G_1 + G_2$, when $\mathcal{B} = \{(0,1), (1,0)\}$;

(ii) the *product* $G_1 \times G_2$, when $\mathcal{B} = \{(1,1)\}$;

(iii) the *strong product* $G_1 * G_2$, when $\mathcal{B} = \{(0,1), (1,0), (1,1)\}$.

(A variety of terms for these particular constructions can be found in the literature.)

The notion of NEPS arises in a natural way when studying spectral properties of graphs obtained by binary operations of the type mentioned above.

2. Let us determine the number of walks of length k in the path P_n with n vertices. The adjacency matrix of P_n is of the form

$$\begin{Vmatrix} 0 & 1 & & & O \\ 1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ O & & & 1 & 0 \end{Vmatrix}.$$

It is known that the eigenvalues of this matrix are $\lambda_i = 2\cos\frac{i\pi}{n+1}$ $(i = 1, \ldots, n)$. It is easy to verify that the numbers $\sqrt{\frac{2}{n+1}}\sin\frac{ij\pi}{n+1}$ $(j = 1, \ldots, n)$ are the coordinates u_{ij} of the normalized eigenvector $\mathbf{u}_i$ belonging to λ_i (see [4]). By Theorem 8 we obtain for the number N_{kn} of walks of length k in P_n the expression

$$N_{kn} = \frac{2^{k+1}}{n+1}\sum_{l=1}^{[\frac{n+1}{2}]}\cot^2\frac{2l-1}{n+1}\frac{\pi}{2}\cos^k\frac{2l-1}{n+1}\pi. \tag{6}$$

This result is related to the following two problems treated in the literature.

1. In [29] the following problem is solved.

Determine the number N_{kn} of all zig-zag lines in the plane which (i) consist of segments of length $\sqrt{2}$ with direction $(\pm 1, 1)^T$, (ii) start from one of the points $(0,0), (0,1), \ldots, (0,k-1)$ and, without leaving the rectangle $0 \le x \le n$, $0 \le y \le k-1$, terminate in one of the points $(n,0), (n,1), \ldots, (n,k-1)$.

This question arises in certain problems of the theory of the function spaces, and the answer is given by (6).

2. A particular result from [11] reads:

The number N_{kn} of ways in which a king can make a series of k moves on a one-dimensional chess board (the board of dimensions $1 \times n$) is given by (6).

This is obvious if we use the concept of a graph corresponding to a chess piece on a given chess-board. The vertices of this graph correspond to the squares of the chess-board and two vertices are adjacent if and only if the piece can proceed from one square to the other in one move. In the case considered the corresponding graph is just the path P_n.

9 Applications to Chemistry

In order to solve the Schrödinger equations for complicated many-electron molecular systems, various approximations are used. In the pioneering days of quantum chemistry (in the 1930s

and 1940s) an approximate method for describing the state of single electrons in conjugated hydrocarbons was developed, known under the name *Hückel molecular orbital theory.*[4]

Within the framework of the Hückel method, the Hamiltonian matrix $H = [h_{ij}]$ is a square matrix of order n, where n is the number of carbon atoms in the molecule. Let these carbon atoms be labelled by $1, 2, \ldots, n$. Then the matrix elements h_{rs} are given by

$$h_{rs} = \begin{cases} \alpha & \text{if } r = s = 1, 2, \ldots, n \\ \beta & \text{if } r \neq s \text{ and the atoms } r \text{ and } s \text{ are chemically bonded} \\ 0 & \text{if } r \neq s \text{ and no chemical bond between the atoms } r \text{ and } s \text{ exists.} \end{cases} \tag{7}$$

The parameters α and β are called the *Coulomb* and the *resonance integral*; in Hückel theory these are assumed to be constants. The approximations imposed by the relations (7) are severe. Therefore it is surprising that the results of the Hückel theory are (at least sometimes) in good agreement with both experimental findings and other, more advanced, theoretical approaches.

Having in mind relations (7), we see that the Hückel Hamiltonian matrix can be presented as

$$H = \alpha I_n + \beta A, \tag{8}$$

where A is a symmetric matrix whose diagonal elements equal 0 and whose off-diagonal elements equal 1 or 0, depending on whether the corresponding atoms are connected or not. In fact A is just the adjacency matrix of the Hückel graph[5]. Equation (8) immediately gives the following result.

Theorem 14. *If λ is an eigenvalue and z an eigenvector of the matrix A, then $\alpha + \beta\lambda$ is an eigenvalue and z is an eigenvector of the matrix H.*

From this theorem it follows that the Hückel molecular orbitals Ψ_j coincide with the eigenvectors z_j of the adjacency matrix of the Hückel graph, that is, $\Psi_j = z_j$. The eigenvalues λ_j of the matrix A and the energies E_j of the corresponding electrons are related simply as

$$E_j = \alpha + \beta\lambda_j.$$

There are exactly n different molecular orbitals, namely the z_j for $j = 1, 2, \ldots, n$.

This important conclusion shows that there is a deep and far-reaching relation between the Hückel molecular orbital theory and graph spectral theory. The Hückel theory provides an important field of application of the graph spectra.

For more information on Hückel theory the interested reader can consult, for example, [6], [28], [18].

[4] *Hydrocarbons* are chemical compounds composed of only two elements - carbon (C) and hydrogen (H). A hydrocarbon is *saturated* if its molecules possess only single bonds. If in a molecule there are also multiple bonds, then the hydrocarbon is *unsaturated*. An important class of unsaturated hydrocarbons are the *conjugated* hydrocarbons, each of whose carbon atoms participates in exactly one double bond. We assume that in a hydrocarbon molecule all carbon atoms have the valency 4 and all hydrogen atoms have the valency 1.

[5] The *Hückel graph* is used for an abbreviated representation of conjugated hydrocarbons. Its vertices represent only the carbon atoms, and all its edges are simple (irrespective of whether the corresponding chemical bonds are single or double). The vertices of a Hückel graph may be of degree 1,2 or 3.

The main contribution of [19] was to establish that the Hückel theory and theory of graph spectra are essentially the same. It was Ivan Gutman who realized this fact during some contacts with me in 1971. The relation between Hückel's theory and theory of graph spectra was noticed earlier in [33], but was poorly used later (see, for example, [40]). However, since [19] was published in a mathematical journal, it has not been cited very much in chemical literature. The chemical community has realized the connection between the two theories after [32] has been published[6] but the fact remains that [19] was the first paper to establish clearly this connection.

In chemistry the problem of determining the algebraic multiplicity of the number 0 in the spectra of bipartite graphs is of interest. It can easily be proved that if the spectrum of the corresponding graph contains at least one number zero, then the molecule cannot have the total electron spin equal to zero, which implies its instability in chemical sense. The wave functions for which $\lambda = 0$ are called "non-bonding molecular orbitals".

Let $\eta(G)$ be the algebraic multiplicity of the eigenvalue 0 in the spectrum of the bipartite graph G. The problem is to find out the connection between the graph structure and the number $\eta(G)$. This connection can be, perhaps, expressed by a set of rules by which we can, after a finite number of steps, determine $\eta(G)$, the spectrum in total being thus left undetermined. (This problem for an arbitrary graph was posed in [4]).

The following theorem appears in [19].

Theorem 15. *If q is the maximal number of mutually non-adjacent edges in a tree G having n vertices, then $\eta(G) = n - 2q$.*

This theorem is an immediate consequence of a statement about the coefficients of the characteristic polynomial of the adjacency matrix of a tree from [37]. It has been generalized in [21] in the following way.

Theorem 16. *If a bipartite graph G with n vertices does not contain any cycle of length $4s$ $(s = 1, 2, \dots)$, then $\eta(G) = n - 2q$, where q is the maximal number of mutually non-adjacent edges in G.*

A general solution of the problem of finding the multiplicity of 0 in the spectrum of a graph is not known, but a variety of partial results have been obtained. As an illustration we present the following statement from [19] (see also [18], Section 8.1).

Theorem 17. *Assume the graph G has a vertex x of degree 1 where x is adjacent to the vertex y. Then the graphs G and $G - x - y$ have equal multiplicity of the number 0 in their spectra, i.e. $\eta(G) = \eta(G - x - y)$.*

10 Spectral graph theory based on the signless Laplacian

In my papers [16], [23], [17], [25], [26], [27] a spectral graph theory based on the signless Laplacian is outlined. Papers [23], [25], [26], [27] are cited very much in the literature (paper

[6] Relations between the coefficients of the characteristic polynomial and the structure of a graph from [37] were denoted here as the *Sachs theorem*, a name which will be used widely afterwards in chemical literature.

[23] over 100 times). As in founding A-theory, it was necessary to establish a number of basic and simple results. We quote here two such results.

1. We consider the enumeration of walks.

In order to introduce a new notion we shall first rephrase the definition of a walk from Section 6.

Definition 6. *A walk (of length k) in an (undirected) graph G is an alternating sequence $v_1, e_1, v_2, e_2, \ldots, v_k, e_k, v_{k+1}$ of vertices $v_1, v_2, \ldots, v_k, v_{k+1}$ and edges $e_1, e_2, \ldots, e_k$ such that for any $i = 1, 2, \ldots, k$ the vertices v_i and v_{i+1} are distinct end-vertices of the edge e_i.*

Such a walk can be imagined as an actual walk of a traveller along the edges in a diagrammatic representation of the graph under consideration. The traveller always walks along an edge from one end-vertex to the other. Suppose now that we allow the traveller to change his mind when coming to the midpoint of an edge: instead of continuing along the edge towards the other end-vertex, he could return to the initial end-vertex and continue as he wishes. Then the basic constituent of a walk is no longer an edge; rather we could speak of a walk as a sequence of *semi-edges*. Such walks could be called *semi-edge walks*. A semi-edge in a walk could be followed by the other semi-edge of the same edge (thus completing the edge) or by the same semi-edge in which case the traveller returns to the vertex at which he started. A formal definition of a semi-edge walk is obtained from the above definition of a walk by deleting the word "distinct" from the description of end-vertices. Hence we have the following definition.

Definition 7. *A semi-edge walk (of length k) in an (undirected) graph G is an alternating sequence $v_1, e_1, v_2, e_2, \ldots, v_k, e_k, v_{k+1}$ of vertices $v_1, v_2, \ldots, v_{k+1}$ and edges $e_1, e_2, \ldots, e_k$ such that for any $i = 1, 2, \ldots, k$ the vertices v_i and v_{i+1} are end-vertices (not necessarily distinct) of the edge e_i.*

In both definitions we shall say that the walk *starts* at the vertex v_1 and *terminates* at the vertex v_{k+1}.

The well known theorem concerning the powers of the adjacency matrix (Theorem 7) has the following counterpart for the signless Laplacian (see [23]).

Theorem 18. *Let Q be the signless Laplacian of a graph G. The (i, j)-entry of the matrix Q^k is equal to the number of semi-edge walks of length k starting at vertex i and terminating at vertex j.*

Proof. For $k = 1$ the statement is obviously true. The result follows by induction on k just as in the proof of the corresponding theorem for the adjacency matrix.

2. The following statement and its proof is analogous to an existing result of mine related to the adjacency spectrum [18, Theorem 3.13]. The proof is taken from [17].

Theorem 19. *Let G be a connected graph of diameter D with e distinct Q–eigenvalues. Then $D \leq e - 1$.*

Proof. By Theorem 18 the (i, j)-entry $q_{i,j}^{(k)}$ of Q^k is the number of semi-edge walks of length k from i to j. By the definition of the diameter, for some vertices i and j there is no semi-edge walk of length k connecting i and j for $k < D$, whereas there is at least one for $k = D$.

Hence we have $q_{i,j}^{(k)} = 0$ for $k < D$ and $q_{i,j}^{(k)} > 0$ for $k = D$. The minimal polynomial of the matrix Q is of degree $e(G) = e$ and yields a recursive relation connecting $e + 1$ consecutive members of the sequence $q_{i,j}^{(k)}$, $k = 0, 1, 2, \ldots$. The assumption $D > e - 1$ would cause that all members of the sequence $q_{i,j}^{(k)}$, $k = 0, 1, 2, \ldots$ are equal to 0 what is impossible. The obtained contradiction proves the theorem.

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