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Endomorphisms of a Weighted Molecular Graph and Its Spectrum

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Abstract

We study the interrelationship between the endomorphisms of a weighted (molecular) graph and its spectral properties. The obtained results are helpful in design of molecular graphs with a given subspectrum and may be of use for materials engineering of substances with tailored electronic and photonic properties.

1 Introduction

A weighted (colored in other terminology) graph is a graph (directed or undirected), to every vertex and every edge of which some quantity (weight) is attached. Weighted graphs naturally appear in chemistry, as molecular graphs [1–5]: here, the weight of a vertex corresponds to the sort of an atom, while the weight of an edge designates the type of a chemical bond. Another opportunity is given by geometrical graphs, where the weight of an edge corresponds to the Euclidean distance between a pair of respective atoms. Usual undirected graphs with or without self-loops comprise a particular case of weighted graphs when the weight is allowed to take on only two values 0 or 1.

It is a well-known fact (see [1–5]) that the spectral properties of molecular graphs have numerous important applications in the theoretical organic, physical and quantum chemistry. Hückel's molecular orbital theory, evaluation of the energy of conjugated molecules, spectral properties of polyhexagonal systems and computations with the characters of symmetry groups of graphs just provide a few impressive examples of such applications.

A lot of correlations are known between the spectrum of a molecular graph and its automorphism group (see [3–5]). In a more general context, such interplay may be investigated with the use of the centralizer algebras of permutation groups [6]. Numerous results in the quantum chemistry can be regarded as the applied theory of representations of finite groups (see [7–9] for the case of the symmetric group).

In the present paper, we shall investigate interrelations between the spectrum of a graph and its generalized symmetries, that is, endomorphisms of graphs. Here, an endomorphism of a graph Γ is a function mapping its vertex set V into V, which preserves edges of Γ. An endomorphism is called strict if it also preserves nonedges of Γ. We associate to a strict endomorphism ε of a weighted graph Γ a certain partition of V and characterize this partition in internal terms of Γ. Our main result is that the existence of classes of this partition, which satisfy certain numerical restrictions, implies the existence of eigenvalues of the adjacency matrix $A = A(\Gamma)$, for multiplicities of which we are giving an efficient lower bound.

In Section 2, all necessary preliminaries are presented, while formulations and proofs of main results are given in Section 3. A short discussion of possible applications of our results and their connections with other investigations in the spectral graph theory and in the theory of semigroups is provided in Section 4.

2 Preliminaries

We recall that a *semigroup* S is a nonempty set with a binary associative operation $\circ$ (see [10]). Usually, for $s_i, s_j \in S$ we write $s_i s_j$ instead of $s_i \circ s_j \in S$.

A *monoid* M is a semigroup with a unity element 1 such that

$$\forall s \in S \qquad 1s = s1 = s.$$

A *group* H is a particular case of a monoid, for which each element $h \in H$ has, in H, its unique inverse h^{-1} such that

$$h^{-1}h = hh^{-1} = 1.$$

An element a of a monoid M is called an *idempotent* if $aa = a^2 = a$. For every element g of a finite monoid M there exists the minimum power m, called *period* of g [10], such that g^m is an idempotent and, moreover,

$$g^m g^r = g^r g^m = g^r \qquad (r_{\min} \leq r \leq r_{\min} + m - 1),$$

where $r_{\min} \geq 0$ is the *index* of g (see [10]). In other words, every such idempotent power g^m serves as a unity for the corresponding cyclic subgroup $K_g = \{g^s, g^{s+1}, \ldots, g^{s+m-1}\}$ $(s = r_{\min})$ generated by $g \in M$.

Any semigroup S can be represented by the endomorphisms of some structure X (see [10]). Herein, we shall consider the endomorphisms of graphs.

Let $\Gamma = (V, E)$ be a *graph* with the *vertex set* V $(|V| = n)$ and the *edge set* E $(|E| = m)$; we consider directed and undirected graphs with and without self-loops. To each edge (i, j) $(1 \leq i, j \leq n)$ we associate a number a_{ij} which is called the *weight* of (i, j). In the case when $i = j$, the number a_{ii} may be interpreted as the weight of a vertex i or of the self-loop lying in the vertex i. Let $A = (a_{ij})_{i,j=1}^n$ be the *adjacency matrix* of a weighted graph Γ. The equality $a_{ij} = 0$ (resp. $a_{ii} = 0$) will be regarded as the absence of the arc (i, j) (loop in a vertex i) in Γ. We denote by A_u and $A^{(u)}$ the u-th row and u-th column of a matrix A, respectively.

An *endomorphism* ε of a graph Γ is an arbitrary function $\varepsilon : V \mapsto V$ which preserves the edges of Γ, i.e., $\varepsilon(E) \subseteq E$. An endomorphism ε is called *strict* if it also preserves the nonedges of Γ, viz.:

$$\forall u, v \in V \qquad (u, v) \in E \Leftrightarrow (\varepsilon(u), \varepsilon(v)) \in E. \tag{1}$$

An analog of the condition (1) for an arbitrary weighted graph Γ can be given in the following matrix form

$$\forall u, v \in V \qquad a_{uv} = a_{\varepsilon(u)\varepsilon(v)}. \tag{2}$$

It is convenient to consider for any endomorphism its "adjacency" matrix $E(\varepsilon) = (e_{ij})_{i,j=1}^n$, where

$$e_{ij} = \begin{cases} 1 & \text{if } j = \varepsilon(i) \\ 0 & \text{otherwise;} \end{cases}$$

$E(\varepsilon)$ can be regarded as the generalization of a permutational matrix (cf [6]). The following simple proposition is a direct analog of a well-known property of a permutational matrix.

Proposition 1. *Let A be the adjacency matrix of a weighted graph Γ and let $\varepsilon : V \mapsto V$ be a function on the vertex set of Γ. Then the function ε is a strict endomorphism of Γ if and only if*

$$E(\varepsilon)A\,(E(\varepsilon))^T = A, \tag{3}$$

where C^T is the transpose of the matrix C.

Note that it easily follows from (3) that the set $\mathrm{End}(\Gamma)$ of all strict endomorphisms of Γ is closed with respect to the composition of functions, that is, forms a semigroup (monoid).

3 Main results

Let Γ be a weighted graph with the vertex set V and the adjacency matrix A. Let $\varepsilon \in E(\Gamma)$ be its arbitrary strict endomorphism. Define the equivalence relation $\sim_\varepsilon$ as follows:

$$u \sim_\varepsilon v \Leftrightarrow \varepsilon(u) = \varepsilon(v) \qquad (\textit{strict equivalency}).$$

Proposition 2. *Let $\varepsilon : V \mapsto V$ be a strict endomorphism of a weighted graph Γ with the adjacency matrix A. Then for each pair u, v of $\sim_\varepsilon$-equivalent points we have that $A_u = A_v$ and $A^{(u)} = A^{(v)}$.*

Proof. Fix an arbitrary $x \in V$. Then $a_{ux} = a_{\varepsilon(u)\varepsilon(x)} = a_{\varepsilon(v)\varepsilon(x)} = a_{vx}$. Thus, $A_u = A_v$. Analogously, $A^{(u)} = A^{(v)}$. □

For each weighted graph Γ with an adjacency matrix A we also define three following equivalence relations:

$$u \sim_r v \Leftrightarrow A_u = A_v \qquad (\textit{row equivalency}),$$
$$u \sim_c v \Leftrightarrow A^{(u)} = A^{(v)} \qquad (\textit{column equivalency}),$$
$$u \sim v \Leftrightarrow u \sim_r v \text{ and } u \sim_c v \qquad (\textit{graph equivalency}).$$

***Remark* 1.** If A is a symmetric, skew-symmetric or Hermitian matrix, then, evidently, all the three relations $\sim_r$, $\sim_c$ and $\sim$ coincide.

Corollary 2.1. *For each strict endomorphism ε of Γ $u \sim_\varepsilon v \Rightarrow u \sim v$, that is, any two strictly-equivalent vertices are also graph-equivalent.*

Corollary 2.2. *If a weighted graph Γ has a noninvertible strict endomorphism, then $\sim$ is a nontrivial equivalence relation on V.*

It turns out that the converse of Corollary 2.2 is also true. First, we need to prove the following

Lemma 3. *Let W_r (resp. W_c) be an equivalence class of $\sim_r$ (resp. $\sim_c$). Then a_{uv} is constant for all $u \in W_r$ and all $v \in W_c$.*

Proof. Let $u, u' \in W_r$ and $v, v' \in W_c$ be arbitrary vertices. Then $A_u = A_{u'}$ and it implies $a_{uv} = a_{u'v}$. Likewise, $A^{(v)} = A^{(v')}$ implies that $a_{u'v} = a_{u'v'}$. Combining these equalities, we obtain $a_{uv} = a_{u'v'}$, as required. □

Theorem 4. *Let Γ be a weighted graph with the vertex set V and the adjacency matrix A. Then Γ has a noninvertible strict endomorphism if and only if $\sim$ is a nontrivial equivalence relation on V.*

Proof. By Corollary 2.2, the existence of a noninvertible endomorphism implies that $\sim$ is nontrivial. Now assume that $\sim$ is nontrivial. Let $T \subseteq V$ be a subset which is a *transversal* of equivalence classes of $\sim$ (in the sense of [11]). In other words, T intersects each equivalence class of $\sim$ by exactly one element. Define a mapping $\varepsilon : V \mapsto T$ by the following rule

$$\forall v \in V, w \in T \qquad \varepsilon(v) = w \Leftrightarrow v \sim w.$$

Then $\varepsilon(v) \sim v$ for each $v \in V$. In particular, $\varepsilon(v) \sim_r v$ and $\varepsilon(v) \sim_c v$. Now, by Lemma 3, we obtain that $a_{uv} = a_{\varepsilon(u)\varepsilon(v)}$, i.e., ε is a strict endomorphism. Since $\varepsilon(V) = T$ and $|T| < |V|$, ε is noninvertible. □

In what follows, any set W of $\sim$-equivalent vertices will be called a set of *twinned* vertices. An equivalence class of $\sim$ is called a maximal set of twinned vertices. If Γ is an undirected graph, then there are two possibilities for a set W of twinned vertices:

$$\begin{array}{lll} \text{either} & a_{uv} = 0, \ \ u, v \in W & (\textit{uncoupled case}) \\ \text{or} & a_{uv} = 1, \ \ u, v \in W & (\textit{coupled case}). \end{array}$$

As we have seen before, for each strict endomorphism ε of Γ there exists $m \in \mathcal{N}$ such that $\sigma = \varepsilon^m$ is an idempotent, that is, $\sigma^2 = \sigma$. Denote by M the set of all idempotents of Γ. For each $\sigma \in M$, $\sigma^2 = \sigma$ and $\sigma(u) \sim_\sigma u$.

Proposition 5. *Let M be the set of all strict idempotent endomorphisms of a weighted graph Γ with the vertex set V and adjacency matrix A. Then we have*

$$\operatorname{rk}(A) \leq \min_{\sigma \in M} |\sigma(V)|, \tag{4}$$

where rk(A) stands for the rank of A; or, equivalently,

$$\eta(A) \geq |V| - \min_{\sigma \in M} |\sigma(V)|, \tag{5}$$

where $\eta(A)$ stands for the nullity of A and $\sigma(V)$ is the image of V with respect to the action of σ.

Proof. Let $\sigma \in M$. As we have seen above, $\sigma(u) \sim_\sigma u$ for all $u \in V$. By Corollary 2.1, it follows that

$$A_{\sigma(u)} = A_u \quad \text{and} \quad A^{(\sigma(u))} = A^{(u)}. \tag{6}$$

Then (6) can be rewritten as follows

$$E(\sigma) \cdot A = A = A \cdot (E(\sigma))^T.$$

Since the rank of the matrix product is not greater than the rank of each factor, we get at that

$$\operatorname{rk}(A) \leq \operatorname{rk}(E(\sigma)) = |\sigma(V)|$$

for each $\sigma \in M$. This implies (4) and, consequently, (5). □

Let $K \subseteq V$ be an arbitrary subset of cardinality k. We say that K is a (k, θ, λ)*-subset of rows of* A if the rank of a submatrix $(A'_w)_{w \in K}$ of the matrix $A' = A - \lambda I$ is $k - \theta$ (where I is the identity matrix).

Lemma 6. *Let $K \subseteq V$ is a (k, θ, λ)-subset of rows of a matrix A and $\theta \geq 1$, then λ is an eigenvalue of A of multiplicity greater or equal than θ.*

Proof. *Set $A' = A - \lambda I$. Among the rows of $(A'_w)_{w \in K}$, we have exactly $k - \theta$ linearly-independent. Consequently, the number of linearly-independent rows of A' is at most $(n-k) + (k-\theta) = n - \theta$. Therefore, $\eta(A') \geq \theta$. Since the multiplicity of the eigenvalue λ of A is at least $\eta(A')$, the multiplicity of λ is at least θ.* □

As a direct consequence of, we get the following

Theorem 7. *Let A be the adjacency matrix of a weighted graph Γ. Assume that there exist $(k_i, \theta_i, \lambda_i)$-subsets W_i of rows of A; $1 \leq i \leq s$. If $\theta_i \geq 1$ for each $1 \leq i \leq s$, then λ_i is an eigenvalue of A, the multiplicity of which is greater or equal than θ_i.*

***Remark* 2.** The same results may be obtained for the sets of columns of A.

***Remark* 3.** If for some set $1 \leq j_1 < j_2 < \cdots < j_k \leq s$ of indices $\lambda = \lambda_{j_1} = \cdots = \lambda_{j_k}$ and the sets $W_{j_1}, W_{j_2}, \ldots, W_{j_k}$ are pairwise disjoint, then the multiplicity of λ is at least $\theta_{j_1} + \theta_{j_2} + \cdots + \theta_{j_k}$.

We will discuss in next section how our two main results (Theorem 4 and Theorem 7) can be combined for practical applications.

4 Discussion

4.1. Strict combinatorial images are very helpful in the consideration of the eigenvalues of graphs. We refer especially to Section 2.3 of [12], where a very useful way of treating the eigenvectors of a graph is presented. One could find in the same book a number of impressive applications of this method.

In our paper, we are trying to attract the reader's attention to some supplementary methods of the investigation of the eigenvalues of graphs. In a few words, our idea is to speculate on the existence of equal lines (that is, rows and columns) in the adjacency matrices of graphs.

Maximal classes of such lines play an important role in the evaluation of the multiplicity of certain eigenvalues of a graph (see examples below). Algebraic interpretation of such classes is similar to that of orbits of the automorphism group of a graph. We suppose that a comparison of two main equivalences (strong and graph) introduced in this paper stresses essential similarities and distinctions between automorphisms and strict endomorphisms. From the other hand, we admit that the consideration of endomorphisms and eigenvalues may be carried out separately and independently of each other.

4.2. To the chemist, evaluation of the multiplicities of the eigenvalues of a molecular graph is a practically important task. Usually, molecular graphs are relatively small and are presented pictorially; therefore, simple tricks demonstrated by us here in a few examples can be rather helpful. These tricks are immediate consequences of the theoretical results developed in the previous section.

Let us detect a few classes of "standard" subgraphs of a graph Γ, the existence of which immediately implies some precise information on eigenvalues. These subgraphs may readily be represented by their adjacency matrices.

***Example* 1.** The hanging star with θ rays, where $\theta = 3$:

$$\begin{bmatrix} \star & 1 & 1 & 1 \\ 1 & \alpha & 0 & 0 \\ 1 & 0 & \alpha & 0 \\ 1 & 0 & 0 & \alpha \end{bmatrix} .$$

Here, $\star$ in the first line stands for an arbitrary loop weight corresponding to the point of attachement of the hanging star to the whole graph, while the entries in the lower lines correspond to three pendant vertices. Existence of such a star contributes exactly $\theta - 1$ linearly-independent eigenvectors which belong to the same eigenvalue $\lambda = \alpha$, where α is the weight of loops in the pendant vertices.

***Example* 2.** Let us consider a subgraph with a cycle of the length four:

$$\begin{bmatrix} \star & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & \star & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \star & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \star & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & \alpha & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & \alpha \end{bmatrix} ,$$

where, the "starred" vertices may have (like in the precedent example) some additional adjacencies, while all the adjacencies of the "unstarred" vertices are shown in the matrix. Two loops in the subgraph have the same weight α. This subgraph contributes to the whole spectrum of Γ at least one eigenvalue α.

In both examples above, we were dealing with the uncoupled twinned vertices. Now consider the coupled twinned vertices.

***Example* 3.** A hanging triangle

$$\begin{bmatrix} \star & 1 & 1 \\ 1 & \alpha & \beta \\ 1 & \beta & \alpha \end{bmatrix},$$

where α and β are again the weights of a loop and edge, respectively, contributes to the spectrum of Γ one eigenvalue $\lambda = \alpha - \beta$.

***Example* 4.** A more complicated subgraph

$$\begin{bmatrix} \star & 1 & 0 & 0 & 0 \\ 1 & \star & 1 & 1 & 1 \\ 0 & 1 & \alpha & \beta & \beta \\ 0 & 1 & \beta & \alpha & \beta \\ 0 & 1 & \beta & \beta & \alpha \end{bmatrix}$$

contributes two eigenvalues $\lambda = \alpha - \beta$.

We invite the reader to construct now his own further examples of similar or even more sophisticated "standard" subgraphs.

4.3. It is worthy to mention that the subsets of the twinned vertices of either kind, in particular, maximal subsets, appear as subgraphs of specific interest in chemistry (especially, in quantum chemistry). For instance, in the above examples, the weight α of a self-loop in vertex i may be interpreted as the value $\alpha = \alpha_i = \int \psi_i H \psi_i^* d\tau$, where α_i is the coulomb integral of an atom i (we refer to the quantum-chemical graph Γ which appear in the Hückel method (see, e.g., [1–5]). A similar interpretation in terms of resonance integrals $\beta_{ij} = \int \psi_i H \psi_j^* d\tau$ works for other, nondiagonal, elements of the adjacency matrix of the Hückel graph. Thus, finally, certain eigenvalues of the Hückel graph and their multiplicities acquire a strict physical explanation.

4.4. There is a number of other significant areas of spectral graph theory which (explicitly or implicitly) are related to the topics in this paper. We would like to give here just a few hints to such interplays.

Idempotent matrices play a significant role in the theory of matrices. In particular, they arise as the projection operators related to the eigenvalues and eigenvectors of a matrix. These applications are presented in [13].

A classical approach in spectral graph theory, which is based on the use of the so-called *divisors of graphs*, describes how some partition of a matrix A into rectangular blocks enables one to find "nonevident" eigenvalues λ of a graph (that is those λ which are not equal to α or $\alpha - \beta$, in terms of the examples above). This approach is presented with all details in [4]; also see [3, 5; 13–15], where other interesting approaches are expounded.

Note that in a more modern terminology divisors of graph correspond to so-called equitable partitions of the vertex set of graphs; see [12]. In [17], this notion is considered in a more wide context of colored (weighted) graphs. An original approach to estimating the multiplicities of the eigenvalues was recently proposed in [16].

To conclude, we would like to stress that the paper [18] by Nummert played an important role in the genesis of the approach presented in this work. In particular, a few of our results are generalizations, to the case of weighted graphs, of corresponding theorems by Nummert.

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