Graph transformations which preserve the multiplicity of an eigenvalue

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Abstract

Graph transformations which preserve the multiplicity of the eigenvalue zero in the spectrum are known since 1970s and are of importance in chemical applications. We now show that analogous transformations hold for all graph eigenvalues that are of the form $2 \cos r\pi$, where r is a rational number, $0 < r < 1$.

1. Introduction

In this paper we consider finite labeled graphs without loops, multiple or directed edges. The set of all such graphs, possessing at least one pair of adjacent vertices, is denoted by $\mathcal{G}_1$. The set of all such graphs, possessing at least one pair of nonadjacent vertices, is denoted by $\mathcal{G}_2$. The set of graphs possessing a bridge is denoted by $\mathcal{G}_3$. The set of disconnected graphs is denoted by $\mathcal{G}_4$. Evidently, $\mathcal{G}_3 \subset \mathcal{G}_1$ and $\mathcal{G}_4 \subset \mathcal{G}_2$. Let G be an N-vertex graph from $\mathcal{G}_1 \cup \mathcal{G}_2$. Let, further, A be the adjacency matrix of G. Then the number λ and the N-dimensional column-vector C (whose components are not all equal to zero), satisfying

$$A\,C = \lambda C, \tag{1}$$

are said to be an eigenvalue and an eigenvector, respectively, of the graph G [2]. If C is written in the form $(C_1, C_2, \ldots, C_N)^t$, then its component C_1 is assumed to be associated with the ith vertex of G.

The eigenspace of A, corresponding to the eigenvalue λ is denoted by $\mathscr{C}(G, \lambda)$. Its dimension $\eta(G, \lambda)$ is the multiplicity of the eigenvalue λ in the spectrum of the graph G.

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Note that if λ is not an eigenvalue of G, then $\mathscr{C}(C, \lambda)$ contains a single element, namely the vector $\mathbf{0} = (0, 0, \ldots, 0)^t$.

The following result is immediate.

Lemma 1. *Let G and G' be two graphs. If a bijection exists between $\mathscr{C}(G, \lambda)$ and $\mathscr{C}(G', \lambda)$, then $\eta(G, \lambda) = \eta(G', \lambda)$.*

In this paper we show that for certain structurally related graphs G and G' and for certain numbers λ the bijection required in Lemma 1 exists for all graphs G from $\mathscr{G}_1$, $\mathscr{G}_2$, $\mathscr{G}_3$ or $\mathscr{G}_4$. Results of this kind have been obtained in the 1970s for the special case of $\lambda = 0$ [3–5,7]; these have far-reaching chemical applications whose details are outlined elsewhere [6, 8, 10]. A closely related study (also concerned solely with the case $\lambda = 0$) was published recently [9].

2. The main results

In what follows r will denote a rational number, $0 < r < 1$. By p and q we denote the mutually prime integers, such that $r = p/q$.

Let $G_1 \in \mathscr{G}_1$. Let x and y be two adjacent vertices of $\mathscr{G}_1$. Construct the graph $G'_n[n]$ bt deleting the edge between x and y, and by joining x and y with the endpoints of an n-vertex path (see Fig. 1).

Theorem 1. *If $\lambda = 2\cos r\pi$, then the equality $\eta(G_1, \lambda) = \eta(G'_1[n], \lambda)$ holds for all $G_1 \in \mathscr{G}_1$, provided (a) p is even and $n = q$, or (b) p is odd and $n = 2q$. The structure of $G'_1[n]$ is shown in Fig. 1.*

Let $G_2 \in \mathscr{G}_2$. Let x and y be two nonadjacent vertices of G_2. Construct the graph $G'_2[n]$ by introducing an edge between x and y, and by joining x and y with the endpoints of an n-vector path (see Fig. 2).

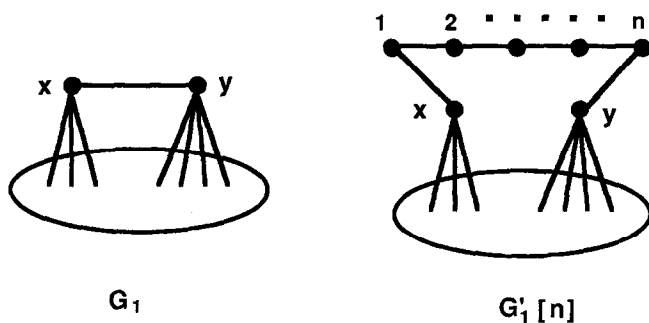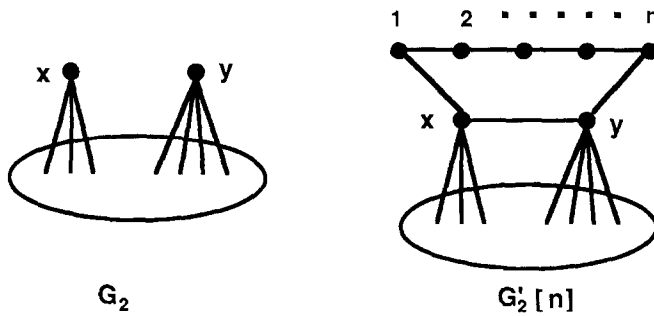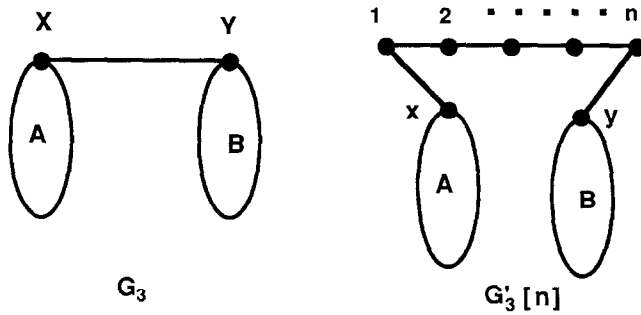$$G_1 \qquad\qquad G'_1[n]$$

Fig. 1.

Fig. 2.

Fig. 3.

Theorem 2. *If* $\lambda = 2\cos r\pi$, *then the equality* $\eta(G_2, \lambda) = \eta(G'_2[n], \lambda)$ *holds for all* $G_2 \in \mathscr{G}_2$, *provided p is odd and* $n = q$. *The structure of* $G'_2[n]$ *is shown in Fig. 2.*

Let $G_3 \in \mathscr{G}_3$. Let x and y be two vertices of G_3, belonging to a bridge. Construct the graph $G'_3[n]$ by deleting the edge between x and y, and by joining x and y with the endpoints of an n-vertex path (see Fig. 3).

Theorem 3. *If* $\lambda = 2\cos r\pi$, *then the equality* $\eta(G_3, \lambda) = \eta(G'_3[n], \lambda)$ *holds for all* $G_3 \in \mathscr{G}_3$, *provided* $n = q$. *The structure of* $G'_3[n]$ *is shown in Fig. 3.*

Let $G_4 \in \mathscr{G}_4$. Let x and y be two vertices of G_4, belonging to different components. Construct the graph $G'_4[n]$ by introducing an edge between x and y, and by joining x and y with the endpoints of an n-vertex path (see Fig. 4).

Theorem 4. *If* $\lambda = 2\cos r\pi$, *then the equality* $\eta(G_4, \lambda) = \eta(G'_4[n], \lambda)$ *holds for all* $G_4 \in \mathscr{G}_4$, *provided* $n = q$. *The structure of* $G'_4[n]$ *is shown in Fig. 4.*
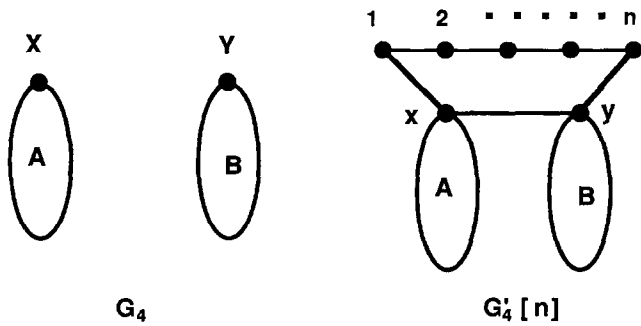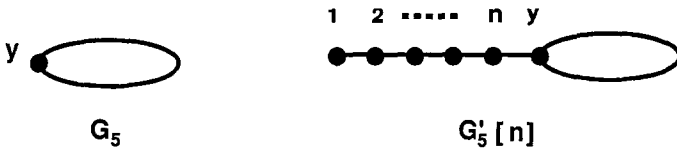
Fig. 4.

Fig. 5.

Table 1

λ	Theorem 1	Theorem 2	Theorem 3	Theorem 4	Theorem 5
$-\sqrt{3}$	$n = 12$	$n = 6$	$n = 6$	$n = 6$	$n = 6$
$-\sqrt{2}$	$n = 8$	$n = 4$	$n = 4$	$n = 4$	$n = 4$
-1	$n = 3$	—	$n = 3$	$n = 3$	$n = 3$
0	$n = 4$	$n = 2$	$n = 2$	$n = 2$	$n = 2$
1	$n = 6$	$n = 3$	$n = 3$	$n = 3$	$n = 3$
$\sqrt{2}$	$n = 8$	$n = 4$	$n = 4$	$n = 4$	$n = 4$
$\sqrt{3}$	$n = 12$	$n = 6$	$n = 6$	$n = 6$	$n = 6$

Let G_5 be a graph with at least one vertex y. Construct the graph $G'_5[n]$ by joining y with an endpoint of an n-vertex path (see Fig. 5).

Theorem 5. *If $\lambda = 2\cos r\pi$, then the equality $\eta(G_5, \lambda) = \eta(G'_5[n], \lambda)$ holds for all graphs G_5, provided $n = q$. The structure of $G'_5[n]$ is shown in Fig. 5.*

Table 1 lists the values of n for some of the most usual choices of λ. Note that for $\lambda = 0$ these values were previously known [3–5, 7], except for the case of Theorem 4. In order to prove the results listed above we need some preparations.

3. An auxiliary polynomial

Define the polynomials $S_k(\lambda)$, $k = -1, 0, 1, \ldots$ in the following recursive manner: $S_{-1}(\lambda) \equiv 0$; $S_0(\lambda) \equiv 1$, for $k \geqslant 1$, $S_k(\lambda) = \lambda S_{k-1}(\lambda) - S_{k-2}(\lambda)$. Hence, $S_1(\lambda) = \lambda$; $S_2(\lambda) = \lambda^2 - 1$; $S_3(\lambda) = \lambda^3 - 2\lambda$; $S_4(\lambda) = \lambda^4 - 3\lambda^2 + 1$, etc. Note that $S_k(\lambda)$ coincides with the characteristic polynomial of the path graph with k vertices. Furthermore, $S_k(\lambda)$ is just one of the standard forms of the Chebyshev polynomial of the first kind [1]. The following two lemmas are well-known results of the theory of Chebyshev functions [1]:

Lemma 2. *If* $\lambda = 2\cos\theta$, *then* $S_k(\lambda) = \sin(k + 1)\theta/\sin\theta$. *Consequently, the zeros of* $S_k(\lambda)$ *are the numbers* $2\cos(j\pi/k + 1)$, $j = 1, 2, \ldots, k$, *each having multiplicity one.*

Lemma 3. *For* $\lambda = 2\cos(j\pi/k + 1)$, $S_{k-1}(\lambda) = (-1)^{j+i}$.

Let G be a graph and $x, 1, 2, \ldots, n, y$ its distinct vertices. Let x be adjacent to 1, i adjacent to $i + 1$, $i = 1, \ldots, n - 1$, and n adjacent to y. The vertices $1, 2, \ldots, n$ are of degree two.

Let λ be an eigenvalue of G and C the corresponding eigenvector. Then from (1) we obtain

$$\lambda C_1 = C_x + C_2, \tag{2a}$$

$$\lambda C_k = C_{k-1} + C_{k+1}, \quad k = 2, \ldots, n - 1, \tag{2b}$$

$$\lambda C_n = C_{n-1} + C_y. \tag{2c}$$

From (2a) and (2b) it immediately follows

$$C_2 = \lambda C_1 - C_x, \qquad C_3 = \lambda C_2 - C_1 = (\lambda^2 - 1)C_1 - \lambda C_x$$

$$C_4 = \lambda C_3 - C_2 = (\lambda^3 - 2\lambda)C_1 - (\lambda^2 - 1)C_x$$

etc. It is now easily verified that

$$C_k = S_{k-1}(\lambda)C_1 - S_{k-2}(\lambda)C_x, \quad k = 1, 2, \ldots, n. \tag{3}$$

4. Proof of Theorem 1

The proofs of Theorems 1–5 are similar. Therefore we describe in detail the demonstration of the validity of Theorem 1 and they only sketch the proofs of the remaining Theorems 2–5.

To show that for a certain value of λ, the spectral multiplicity of λ is the same for G_1 and $G_1'[n]$, we have to establish a bijection between $\mathscr{C}(G_1, \lambda)$ and $\mathscr{C}(G_1'[n], \lambda)$. Let the eigenvectors $C \in \mathscr{C}(G_1, \lambda)$ and $C' \in \mathscr{C}(G_1'[n], \lambda)$ correspond to each other. We choose

C' so that its components which are associated with the vertices of G_1 are the same as in C. Thus, by definition, C' is mapped to a unique element of $\mathscr{C}(G_1, \lambda)$.

The vertices of $G_1[n]$ that are not vertices of G_1 are labeled by $1, 2, \dots, n$ (see Fig. 1). The respective components of C' are $C_1, C_2, \dots, C_n$ and they must satisfy the boundary conditions

$$C_1 = C_y \tag{4a}$$

and

$$C_n = C_x. \tag{4b}$$

In addition to this, $C_1, C_2, \dots, C_n$ must conform to the relations (3).

From (3) and (4) we see that $C_1, C_2, \dots, C_n$ are fully determined by means of C_x and C_y. This implies that C' is the unique element of $\mathscr{C}(G_1[n], \lambda)$ on which C is mapped, provided that the conditions (3) and (4) can simultaneously be fulfilled.

Now, in order to put (3) and (4) in harmony, we must have

$$S_{k-1}(\lambda)C_1 - S_{k-2}(\lambda)C_x = C_y \quad \text{for } k = 1, \tag{5a}$$

and

$$S_{k-1}(\lambda)C_1 - S_{k-2}(\lambda)C_x = C_x \quad \text{for } k = n. \tag{5b}$$

Condition (5a) is satisfied in a trivial manner. On the other hand, (5b) will hold (as an identity) only if

$$S_{n-1}(\lambda) = 0$$

and

$$S_{n-2}(\lambda) = -1. \tag{6b}$$

From Lemmas 2 and 3 we see that (6a) implies $\lambda = 2\cos(j\pi/n)$ whereas (6b) implies that j must be even. If λ has these two properties, then a one-to-one correspondence exists between C and C', resulting in $\eta(G_1, \lambda) = \eta(G_1'[n], \lambda)$.

It remains to establish the value of n. If $\lambda = 2\cos r\pi$ and $r = p/q, (p, q) = 1$, then we have to distinguish between two cases. If p is even, then the choice $n = q$ meets the above established requirements. If p is odd, then by presenting r as $2p/(2q)$ we see that the smallest satisfactory value of n is $2q$.

This completes the proof of Theorem 1. $\square$

5. Proofs of Theorem 2–5

Proof of Theorem 2. The reasoning is analogous as in the case of Theorem 1, except that instead of (4a) and (4b) the boundary conditions read:

$$C_1 = -C_y \quad \text{and} \quad C_n = -C_x.$$

Consequently, instead of (6a) and (6b), λ must satisfy the conditions

$$S_{n-1}(\lambda) = 0 \quad \text{and} \quad S_{n-2}(\lambda) = 1$$

which means that λ must be of the form $2\cos(j\pi/n)$ and j must be odd.

A noteworthy difference between Theorems 1 and 2 is that if $\lambda = 2\cos r\pi$, $r = p/q$ and p is even, then there is no value of n for which $\eta(G_2, \lambda) = \eta(G'_2[n], \lambda)$ would hold for all $G_2 \in \mathscr{G}_2$. $\square$

Proof of Theorem 3. If G_3 has the structure shown in Fig. 3, then in addition to the boundary conditions (4a) and (4b) we have another option, namely

$$C_1 = C_y \tag{7a}$$

and

$$C_n = -C_x. \tag{7b}$$

The eigenvector C' constructed by means of (7a) and (7b) has the following property: Its components associated with the vertices of the subgraph A are equal to the respective components of C. Its components associated with the vertices of the subgraph B are equal to the respective components of $-C$. The only connection between the subgraphs A and B goes via the vertices x and y (see Fig. 3). Therefore, if the relations (3) and (7) can be simultaneously satisfied we will arrive at a correct eigenvector C'. From (3) and (7) it is then concluded that λ must be of the form $2\cos(j\pi/n)$ with j being odd. From (3) and (4) follows that j also can be even, i.e. j can assume any integer value in the interval $[1, n-1]$. $\square$

Proof of Theorem 4. Fully analogous to the proof of Theorem 3.

Proof of Theorem 5. In the case of the graph $G_5[n]$ (see Fig. 5), Eqs. (2a) and (3) remain valid if one sets $C_x = 0$. An easy calculation yields then to $C_k = [S_{k-1}(\lambda)/S_n(\lambda)]C_y$, $k = 1, 2, \ldots, n$. The boundary condition is $C_n = 0$ which is satisfied if $S_{n-1}(\lambda) = 0$ and $S_n = (\lambda) \neq 0$. Hence, $\lambda = 2\cos(j\pi/n)$, $0 < j < n$. $\square$

6. Discussion

Theorems 1–5 can be understood as methods by which a given graph can be transformed into a simpler graph, without influencing the multiplicity of a certain graph eigenvalue. Whereas the first findings of this kind were obtained for the eigenvalue zero, we now showed that analogous results hold for an infinite number of eigenvalues. Our study, however, revealed that the eigenvalues for which the general reduction methods apply must have the peculiar algebraic form $2\cos r\pi$. Whether general multiplicity-preserving graph transformations exist also for other eigenvalues, especially for those greater than or equal to two, remains an open question.

Theorem 3 has the following extension. Let A and B be two graphs with disjoint vertex sets. Let $x_1, x_2, \ldots, x_m$ and $y_1, y_2, \ldots, y_m$ be distinct vertices of A and B, respectively. Construct the graph $G_{3,m}$ by joining x_1 with y_1, $i = 1, 2, \ldots, m$. Construct the graph $G'_{3,m}[n]$ by joining x_1 and y_1 to the endpoints of an n-vertex path, and repeating this for all $i = 1, 2, \ldots, m$. Note that for $m = 1$, the graphs $G_{3,m}$ and $G'_{3,m}[n]$ reduce to the graphs G_3 and $G'_3[n]$, respectively, considered in Theorem 3.

Corollary 3.1. *The statement of Theorem 3 remains valid if the symbols G_3 and $G'_3[n]$ are replaced by $G_{3,m}$ and $G'_{3,m}[n]$, respectively, for any $m \geqslant 1$.*

The special case of the above Corollary for $\lambda = 0$ is a result previously reported in the chemical literature [5, 10].

Acknowledgements

References

[1] M. Abramovitz and I.A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1965).
[2] D. Cvetković, M. Doob and H. Sachs, Spectra of Graphs – Theory and Application (Academic Press, New York, 1980).
[3] D.M. Cvetković and I. Gutman, The algebraic multiplicity of the number zero in the spectrum of a bipartite graph, Mat. Vesnik (Beograd) 9 (1972) 141–150.
[4] D. Cvetković, I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. II, Croat. Chem. Acta 44 (1972) 365–374.
[5] D. Cvetković, I. Gutman and N. Trinajstić, Graphical studies on the relations between the structure and reactivity of conjugated systems: The role of non-bonding molecular orbitals, J. Mol. Struct. 28 (1975) 289–303.
[6] A. Graovac, I. Gutman and N. Trinajstić, Topological Approach to the Chemistry of Conjugated Molecules (Springer, Berlin, 1977).
[7] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. IV. Further application of Sachs formula, Croat. Chem. Acta 45 (1973) 423–429.
[8] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals, Top. Curr. Chem. 42 (1973) 49–93.
[9] D.J. Klein and A.T. Balaban, Generalized Hückel–Möbius rule. J. Mol. Struct. (Theochem) 259 (1992) 307–315.
[10] N. Trinajstić, Chemical Graph Theory (CRC Press, Boca Raton, 1983).