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Eigenvalues of Graphs with Threefold Symmetry

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In many cases, the spectrum of one graph contains the entire spectrum of a second, smaller graph. The larger (composite) graph and the smaller (component) graph are said to be subspectral. Rules are given for constructing two subspectral components of a composite graph which has threefold symmetry such that the eigenvalues of one component and the eigenvalues of the second component taken twice comprise the complete spectrum of the composite graph. The mathematical basis for these rules is shown to be a unitary transformation upon the eigenvalue equation of the adjacency matrix of the composite graph by the matrix which represents threefold rotation.

Key words: Graphs, threefold symmetric, eigenvalues of ~

1. Introduction

Graph theory has been shown to be an appropriate tool for the analysis of topologically-related molecular properties [1]. When applied to the study of conjugated hydrocarbons, a graph theoretical treatment is fully equivalent to a simple Hückel molecular orbital (HMO) treatment [2–4], since the Hückel parameters for such molecules depend only on the adjacency relationships between and among the atoms. In particular, the HMO energy levels for a molecule of this type are identical to the eigenvalues of the adjacency matrix of the graph which has the same pattern of connectedness as the molecule.

In examining tabulated eigenvalues [5], it can be seen that, in many cases, the entire spectrum of one graph is contained in the spectrum of a second, larger graph. In such a case, the larger (composite) graph and the smaller (component) graph are said to be subspectral [6]. Whether such a relationship has any significance for the properties of the corresponding conjugated molecules is uncertain

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[7]. In any case, this sharing of eigenvalues is a curious phenomenon which has been previously noted by others who have provided explanations for its occurrence in several special structural classes [6, 8–11]. A procedure is given here for constructing the subspectral components of a composite graph which possesses threefold symmetry.

2. Construction of the Component Graphs

Consider a graph G characterized by a threefold rotational operation which defines three equivalent sets of vertices **r**, **s**, and **t**, and possibly a self-equivalent vertex **q** lying on the axis of rotation. The following rules may be used to construct two graphs, G_a and G_e, such that the eigenvalues of G_a and the eigenvalues of G_e taken twice comprise the full spectrum of G.

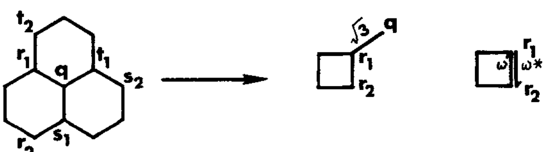
1. First, the vertices in set **r** are drawn, together with all the edges connecting members of the set. Then the vertices through which **r** is connected to **s**, **t**, and possibly **q** (the bridging vertices of **r**) are examined in G.

2. If a bridging vertex $\mathbf{r}_1$ is connected to a vertex $\mathbf{t}_2$ which is symmetry-equivalent to a second bridging vertex $\mathbf{r}_2$, then the weight of the undirected edge between $\mathbf{r}_1$ and $\mathbf{r}_2$ in G (+1 if they are adjacent, zero if they are not) is increased by one unit in G_a. In G_e, the weight of the directed edge from $\mathbf{r}_2$ to $\mathbf{r}_1$ is increased by $\omega = \exp(2\pi i/3)$, and the weight of the directed edge from $\mathbf{r}_1$ to $\mathbf{r}_2$ is increased by $\omega^* = \exp(-2\pi i/3)$. Furthermore, if these directed edges do not belong to a cycle in G_e, they may be replaced by an undirected edge whose weight is equal to the square root of the product of the weights of the directed edges, i.e. either $\sqrt{\omega\omega^*} = 1$ or $\sqrt{(1 + \omega)(1 + \omega^*)} = 1$. (An explanation of the last statement is given in an appendix.)

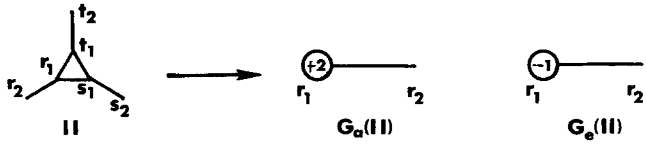
3. If a bridging vertex $\mathbf{r}_1$ is connected to its own symmetry partners $\mathbf{s}_1$ and $\mathbf{t}_1$ in G, then $\mathbf{r}_1$ is weighted +2 in G_a and $(\omega + \omega^*) = -1$ in G_e.

4. If $\mathbf{r}_1$ is connected to **q** in G, then the weight of the undirected edge between $\mathbf{r}_1$ and **q** is $\sqrt{3}$ in G_a; in G_e, this edge and the vertex **q** are omitted.

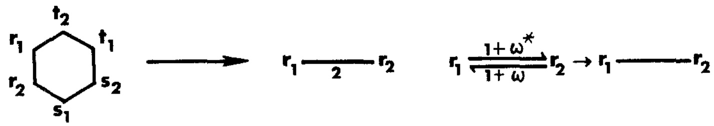
The application of these rules may be illustrated by the following examples.



I $\quad$ G_a(I) $\quad$ G_e(I)



II $\quad$ G_a(II) $\quad$ G_e(II)



III G$_a$(III) G$_e$(III)

The bridging vertices in **I**, **II**, and **III** and the weighted edges and vertices of their respective component graphs have been labelled.

3. Proof

The rules for constructing the subspectral components of a composite graph having threefold symmetry originate in the symmetry properties of the adjacency matrix of the composite graph.

Consider a threefold-symmetric composite graph which contains $3N$ vertices, N vertices in each of the equivalent sets **r**, **s**, and **t**. (Exclude, for the present, any graph containing a vertex **q** on the axis of rotation.) Let such a graph be denoted by G_1. If the vertices of G_1 are numbered in such a way that the number assigned to each vertex in **s** is N greater than the number assigned to its symmetry partner in **r** and N less than the number assigned to its symmetry partner in **t**, then the adjacency matrix of G_1 has the form

$$A(G_1) = \begin{pmatrix} \boldsymbol{B}_1 & \boldsymbol{B}_2 & \boldsymbol{B}_3 \\ \boldsymbol{B}_3 & \boldsymbol{B}_1 & \boldsymbol{B}_2 \\ \boldsymbol{B}_2 & \boldsymbol{B}_3 & \boldsymbol{B}_1 \end{pmatrix}.$$

The elements of the symmetric submatrix $\boldsymbol{B}_1$ represent the adjacency relationships within a single set, **r**, **s**, or **t**; the elements of $\boldsymbol{B}_2$ and $\boldsymbol{B}_3 = (\boldsymbol{B}_2)^T$ represent the adjacency relationships between **r** and **s**, **r** and **t**, and **s** and **t**.
The eigenvalue equation for $A(G_1)$ is

$$A(G_1)\begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{v} \\ \boldsymbol{w} \end{pmatrix} = \varepsilon \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{v} \\ \boldsymbol{w} \end{pmatrix}.$$

A unitary transformation on $A(G_1)$ and its eigenvector may be performed by the matrix which represents the threefold rotational operation:

$$C_3 = \begin{pmatrix} \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \omega\mathbf{1} \\ \mathbf{0} & \omega^*\mathbf{1} & \mathbf{0} \end{pmatrix} = C_3{}^\dagger$$

where $\omega = \exp(2\pi i/3)$. The transformed eigenvalue equation is

$$C_3{}^\dagger A(G_1) C_3 C_3{}^\dagger \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{v} \\ \boldsymbol{w} \end{pmatrix} = \varepsilon C_3{}^\dagger \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{v} \\ \boldsymbol{w} \end{pmatrix}$$

or

$$\begin{pmatrix} B_1 & \omega^* B_3 & \omega B_2 \\ \omega B_2 & B_1 & \omega^* B_3 \\ \omega^* B_3 & \omega B_2 & B_1 \end{pmatrix} \begin{pmatrix} u \\ \omega w \\ \omega^* v \end{pmatrix} = \varepsilon \begin{pmatrix} u \\ \omega w \\ \omega^* v \end{pmatrix}$$

where the identities $\omega^2 = \omega^*$, $(\omega^*)^2 = \omega$, and $\omega\omega^* = 1$ have been employed.

Performance of the matrix multiplication gives three equations:

$$B_1 u + (\omega^* B_3)(\omega w) + (\omega B_2)(\omega^* v) = \varepsilon u, \tag{1}$$
$$(\omega B_2) u + B_1(\omega w) + (\omega^* B_3)(\omega^* v) = \varepsilon \omega w, \tag{2}$$
$$(\omega^* B_3) u + (\omega B_2)(\omega w) + B_1(\omega^* v) = \varepsilon \omega^* v. \tag{3}$$

These equations may be combined in several ways. The linearly independent combinations (1) + ω^*(2) + ω(3), (1) + ω(2) + ω^*(3), and (1) + (2) + (3) lead respectively to Eqs. (4), (5), and (6):

$$(B_1 + B_2 + B_3)(u + v + w) = \varepsilon(u + v + w), \tag{4}$$
$$(B_1 + \omega^* B_2 + \omega B_3)(u + \omega^* w + \omega v) = \varepsilon(u + \omega^* w + \omega v), \tag{5}$$
$$(B_1 + \omega B_2 + \omega^* B_3)(u + \omega w + \omega^* v) = \varepsilon(u + \omega w + \omega^* v). \tag{6}$$

Clearly, the N eigenvalues of the matrix $(B_1 + B_2 + B_3)$, the N eigenvalues of $(B_1 + \omega^* B_2 + \omega B_3)$, and the N eigenvalues of $(B_1 + \omega B_2 + \omega^* B_3)$ together constitute the complete spectrum of $A(G_1)$. Furthermore, since Eq. (6) is the complex conjugate of Eq. (5) and ε is real, the eigenvalues of the matrices $(B_1 + \omega^* B_2 + \omega B_3)$ and $(B_1 + \omega B_2 + \omega^* B_3)$ are identical. Thus the graphs which have as their respective adjacency matrices $(B_1 + B_2 + B_3) = B_a$ and $(B_1 + \omega B_2 + \omega^* B_3) = B_e$ are the subspectral components of G_1.

The relationship between the form of B_a and B_e and the rules for constructing the component graphs $G_{a,1}$ and $G_{e,1}$ may be clarified by means of the following examples. Consider first the benzene graph (**III**) and its adjacency matrix

$$A(\mathbf{III}) = \begin{pmatrix} 01 & 00 & 01 \\ 10 & 10 & 00 \\ 01 & 01 & 00 \\ 00 & 10 & 10 \\ 00 & 01 & 01 \\ 10 & 00 & 10 \end{pmatrix} = \begin{pmatrix} B_1 & B_2 & B_3 \\ B_3 & B_1 & B_2 \\ B_2 & B_3 & B_1 \end{pmatrix}.$$

Notice that $(B_1)_{12} = (B_1)_{21} = 1$, since $\mathbf{r}_1$ is adjacent to $\mathbf{r}_2$, and that $(B_2)_{21} = (B_3)_{12} = 1$, since $\mathbf{r}_1$ is adjacent to $\mathbf{t}_2$ and $\mathbf{r}_2$ to $\mathbf{s}_1$. Thus, B_a and B_e have the form

$$B_a = (B_1 + B_2 + B_3) = \begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix}$$

$$B_e = (B_1 + \omega B_2 + \omega^* B_3) = \begin{pmatrix} 0 & 1 + \omega^* \\ 1 + \omega & 0 \end{pmatrix}.$$

These matrices can be considered adjacency matrices for the edge-weighted graphs $G_a(\mathbf{III})$ and $G_e(\mathbf{III})$.

As a second example, the graph **II** has the adjacency matrix

$$A(\mathbf{II}) = \begin{pmatrix} 01 & 10 & 10 \\ 10 & 00 & 00 \\ 10 & 01 & 10 \\ 00 & 10 & 00 \\ 10 & 10 & 01 \\ 00 & 00 & 10 \end{pmatrix} = \begin{pmatrix} \boldsymbol{B}_1 & \boldsymbol{B}_2 & \boldsymbol{B}_3 \\ \boldsymbol{B}_3 & \boldsymbol{B}_1 & \boldsymbol{B}_2 \\ \boldsymbol{B}_2 & \boldsymbol{B}_3 & \boldsymbol{B}_1 \end{pmatrix}.$$

The nonzero elements of $\boldsymbol{B}_1$ are $(\boldsymbol{B}_1)_{12} = (\boldsymbol{B}_1)_{21} = 1$, since $\mathbf{r}_1$ is connected to $\mathbf{r}_2$; the nonzero elements of $\boldsymbol{B}_2$ and $\boldsymbol{B}_3$ are $(\boldsymbol{B}_2)_{11} = (\boldsymbol{B}_3)_{11} = 1$, because $\mathbf{r}_1$ is connected to both $\mathbf{s}_1$ and $\mathbf{t}_1$. $\boldsymbol{B}_a$ and $\boldsymbol{B}_e$ are therefore given by

$$\boldsymbol{B}_a = (\boldsymbol{B}_1 + \boldsymbol{B}_2 + \boldsymbol{B}_3) = \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\boldsymbol{B}_e = (\boldsymbol{B}_1 + \omega\boldsymbol{B}_2 + \omega^*\boldsymbol{B}_3) = \begin{pmatrix} \omega + \omega^* & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ 1 & 0 \end{pmatrix}.$$

Again, these may be considered the adjacency matrices of the vertex-weighted graphs $G_a(\mathbf{II})$ and $G_e(\mathbf{II})$. The origin of rules (1) through (3) for constructing the component graphs of composite graphs of the form of G_1 should now be apparent.

Suppose the composite graph of interest is identical to a graph of the form of G_1 except that it contains an additional vertex $\mathbf{q}$ which lies on the axis of rotation; let this graph be denoted by G_2. The adjacency matrix of G_2 can be written in the form

$$A(G_2) = \begin{pmatrix} 0 & \boldsymbol{D} & \boldsymbol{D} & \boldsymbol{D} \\ \boldsymbol{D}^T & \boldsymbol{B}_1 & \boldsymbol{B}_2 & \boldsymbol{B}_3 \\ \boldsymbol{D}^T & \boldsymbol{B}_3 & \boldsymbol{B}_1 & \boldsymbol{B}_2 \\ \boldsymbol{D}^T & \boldsymbol{B}_2 & \boldsymbol{B}_3 & \boldsymbol{B}_1 \end{pmatrix}.$$

The nonzero element of the $1 \times N$ vector $\boldsymbol{D}$ represents the edge between $\mathbf{q}$ and each of the sets $\mathbf{r}$, $\mathbf{s}$, and $\mathbf{t}$; the elements of the $N \times N$ submatrices $\boldsymbol{B}_1$. $\boldsymbol{B}_2$, and $\boldsymbol{B}_3$ represent the adjacency relationships within and among the sets $\mathbf{r}$, $\mathbf{s}$, and $\mathbf{t}$, as previously described.

The matrix representing threefold rotation must now be written as

$$\boldsymbol{C}_3' = \begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \omega\mathbf{1} \\ \mathbf{0} & \mathbf{0} & \omega^*\mathbf{1} & \mathbf{0} \end{pmatrix} = (\boldsymbol{C}_3')^\dagger,$$

since rotation about the threefold axis leaves $\mathbf{q}$ unaffected. The eigenvalue equation for $A(G_2)$,

$$A(G_2)\begin{pmatrix} p \\ \boldsymbol{u} \\ \boldsymbol{v} \\ \boldsymbol{w} \end{pmatrix} = \varepsilon \begin{pmatrix} p \\ \boldsymbol{u} \\ \boldsymbol{v} \\ \boldsymbol{w} \end{pmatrix}$$

(where p is the coefficient of the vertex $\mathbf{q}$), becomes under unitary transformation:

$$\begin{pmatrix} 0 & \boldsymbol{D} & \omega^*\boldsymbol{D} & \omega\boldsymbol{D} \\ \boldsymbol{D}^T & \boldsymbol{B}_1 & \omega^*\boldsymbol{B}_3 & \omega\boldsymbol{B}_2 \\ \omega\boldsymbol{D}^T & \omega\boldsymbol{B}_2 & \boldsymbol{B}_1 & \omega^*\boldsymbol{B}_3 \\ \omega^*\boldsymbol{D}^T & \omega^*\boldsymbol{B}_3 & \omega\boldsymbol{B}_2 & \boldsymbol{B}_1 \end{pmatrix}\begin{pmatrix} p \\ \boldsymbol{u} \\ \omega\boldsymbol{w} \\ \omega^*\boldsymbol{v} \end{pmatrix} = \varepsilon \begin{pmatrix} p \\ \boldsymbol{u} \\ \omega\boldsymbol{w} \\ \omega^*\boldsymbol{v} \end{pmatrix}.$$

Performance of the multiplication gives

$$\boldsymbol{D}\boldsymbol{u} + (\omega^*\boldsymbol{D})(\omega\boldsymbol{w}) + (\omega\boldsymbol{D})(\omega^*\boldsymbol{v}) = \varepsilon p \tag{7}$$

$$\boldsymbol{D}^T p + \boldsymbol{B}_1\boldsymbol{u} + (\omega^*\boldsymbol{B}_3)(\omega\boldsymbol{w}) + (\omega\boldsymbol{B}_2)(\omega^*\boldsymbol{v}) = \varepsilon\boldsymbol{u} \tag{8}$$

$$\omega\boldsymbol{D}^T p + (\omega\boldsymbol{B}_2)\boldsymbol{u} + \boldsymbol{B}_1(\omega\boldsymbol{w}) + (\omega^*\boldsymbol{B}_3)(\omega^*\boldsymbol{v}) = \varepsilon\omega\boldsymbol{w} \tag{9}$$

$$\omega^*\boldsymbol{D}^T p + (\omega^*\boldsymbol{B}_3)\boldsymbol{u} + (\omega\boldsymbol{B}_2)(\omega\boldsymbol{w}) + \boldsymbol{B}_1(\omega^*\boldsymbol{v}) = \varepsilon\omega^*\boldsymbol{v}. \tag{10}$$

Once again, Eqs. (8) through (10) may be combined in several ways. Consider first a simplified form of Eq. (7) and the linear combination (8) + ω^*(9) + ω(10):

$$\boldsymbol{D}(\boldsymbol{u} + \boldsymbol{v} + \boldsymbol{w}) = \varepsilon p$$

$$3\boldsymbol{D}^T p + (\boldsymbol{B}_1 + \boldsymbol{B}_2 + \boldsymbol{B}_3)(\boldsymbol{u} + \boldsymbol{v} + \boldsymbol{w}) = \varepsilon(\boldsymbol{u} + \boldsymbol{v} + \boldsymbol{w}). \tag{11}$$

From (7) and (11) can be reconstructed the matrix equation

$$\begin{pmatrix} 0 & \boldsymbol{D} \\ 3\boldsymbol{D}^T & \boldsymbol{B}_1 + \boldsymbol{B}_2 + \boldsymbol{B}_3 \end{pmatrix}\begin{pmatrix} p \\ \boldsymbol{u} + \boldsymbol{v} + \boldsymbol{w} \end{pmatrix} = \varepsilon\begin{pmatrix} p \\ \boldsymbol{u} + \boldsymbol{v} + \boldsymbol{w} \end{pmatrix}$$

which implies that $(N + 1)$ of the $(3N + 1)$ eigenvalues of G_2 are also eigenvalues of a graph $G_{a,2}$ which has as its adjacency matrix

$$\begin{pmatrix} 0 & \boldsymbol{D} \\ 3\boldsymbol{D}^T & \boldsymbol{B}_1 + \boldsymbol{B}_2 + \boldsymbol{B}_3 \end{pmatrix}.$$

It is evident from the form of this matrix that $G_{a,2}$ is identical to $G_{a,1}$ except that the former contains a directed edge of weight 3 from an $\mathbf{r}$ vertex to $\mathbf{q}$ and a directed edge of unit weight from $\mathbf{q}$ to the $\mathbf{r}$ vertex. Since these directed edges between $\mathbf{r}$ and $\mathbf{q}$ do not belong to a cycle in $G_{a,2}$ only the product of their weights is of interest (see Appendix), and therefore they may be replaced by two directed edges weighted $\sqrt{3}$ each, or, equivalently, by a single undirected edge weighted $\sqrt{3}$.

Consider next a second, linearly independent combination of Eqs. (8) through (10), (8) + (9) + (10):

$$(1 + \omega + \omega^*)\boldsymbol{D}^T p + (\boldsymbol{B}_1 + \omega \boldsymbol{B}_2 + \omega^* \boldsymbol{B}_3)(\boldsymbol{u} + \omega \boldsymbol{w} + \omega^* \boldsymbol{v}) = \varepsilon(\boldsymbol{u} + \omega \boldsymbol{w} + \omega^* \boldsymbol{v}). \tag{12}$$

Since $(\omega + \omega^*) = -1$, Eq. (12) reduces to Eq. (6); the second subspectral component of G_2 has as its adjacency matrix $(\boldsymbol{B}_1 + \omega\boldsymbol{B}_2 + \omega^*\boldsymbol{B}_3) = \boldsymbol{B}_e$ and is therefore identical to $G_{e,1}$. Rules (1) through (4) for constructing the subspectral components of a composite graph of the form of G_2 follow immediately from this analysis.

4. Conclusion

It should be noted that the mathematical manipulations employed here can be applied to the treatment of graphs which have other kinds of rotational symmetry. By numbering the vertices of such graphs in a manner consistent with their symmetry properties, and by choosing an appropriate matrix by which to perform the unitary transformation, rules may easily be developed for constructing all the subspectral components of the symmetric composite graphs of interest. In fact, the rules given in [11] for constructing the components of graphs having twofold symmetry arise from matrix manipulations which represent a special case of a unitary transformation by $\boldsymbol{C}_2 = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix}$, since $\boldsymbol{C}_2$ commutes with $A(G)$ in that particular case. Those rules, not originally applicable to a graph which contains one or more vertices lying on the C_2 axis or plane of symmetry, can now be extended to graphs of that form by a treatment analogous to the one used in the second part of Sect. 3 of this paper. (The subspectral components constructed by the extended rules are identical to McClelland's A- and B-fragments for such a graph.) The general treatment presented here should prove useful for the further investigation of graph spectral regularities.

Appendix

By definition, the characteristic determinant of an $N \times N$ adjacency matrix is the sum of $N!$ products of the form $a_{1j_1}a_{2j_2}\cdots a_{Nj_N}$; that is,

$$\det(A - x1) = \sum_{\sigma} (\text{sign } \sigma) a_{1j_1}\cdots a_{Nj_N}$$

where σ represents some permutation $(j_1 j_2 \cdots j_N)$ of the N elements $(1\ 2 \cdots N)$ and sign $\sigma = \pm 1$, according to the parity of the permutation.

Clearly, a given product $a_{1j_1}a_{2j_2}\cdots a_{Nj_N}$ is nonzero if and only if every element a_{ij_i} is nonzero, that is, if and only if there is a directed edge from vertex i to vertex j_i $(i \neq j_i)$ in the graph described by A. (Recall that all diagonal elements a_{ii} are equal to $-x$.)

Suppose that the graph of interest contains a pair of weighted directed edges between vertices k and m. If these edges do not belong to a cycle, then the characteristic determinant of A will contain a nonzero term of the form[1] $a_{1j_1}a_{2j_2}\cdots$

[1] See the discussion of Graovac *et al.* on page 19 of Ref. [12].

$a_{km}a_{mk}\cdots a_{Nj_N}$. Since the numerical value of this product is $a_{km}a_{mk}$, one may substitute for the original directed edges between vertices k and m a pair of directed edges weighted $\sqrt{a_{km}a_{mk}}$ each or, equivalently, a single *undirected* edge weighted $\sqrt{a_{km}a_{mk}}$, without affecting the value of $\det(A - x\mathbf{1})$ or, consequently, the eigenvalues of A.

If, on the other hand, the directed edges between vertices k and m do belong to a cycle, then the expansion of the characteristic determinant of A will contain two additional nonzero terms of the form $a_{12}a_{23}\cdots a_{km}\cdots a_{N1}$ and $a_{1N}\cdots a_{mk}\cdots a_{32}a_{21}$, corresponding to clockwise and counterclockwise circulations about the cycle. In this case, a_{km} and a_{mk} contribute individually to terms in the characteristic polynomial, and therefore there can be no substitutions for the original weighted edges.

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