match no. 21 pp. 81-91 1986

ON HERMITIAN MATRICES ASSOCIATED WITH THE MATCHING POLYNOMIALS OF GRAPHS. PART III.*

THE MATCHING POLYNOMIALS OF BICYCLIC AND TRICYCLIC CATA-CONDENSED GRAPHS ARE THE CHARACTERISTIC POLYNOMIALS OF HERMITIAN MATRICES WITH QUATERNIONIC WEIGHTS.

Ante Graovac** and Oskar E. Polansky

Max-Planck-Institut für Strahlenchemie, D-4330 Mülheim a. d. Ruhr

(Received: September 1986)

ABSTRACT

Using quaternionic edge weights Hermitian weight matrices are derived for bicyclic and tricyclic cata-condensed graphs. They may be adapted to any graph of this type. It is shown how these matrices are used in computer assisted calculations of the eigenvalues of the matching polynomials of the respective graphs.

The connectivity of vertices in a graph G is described by the adjacency matrix $\underline{A} = \underline{A}(G)$ of G. $\underline{A}$ is an nxn symmetrical matrix where n stands for the number of vertices in G. The characteristic polynomial $\Phi(x)$ of G is defined by [4]:

$$\Phi(G) \equiv \Phi(G;x) = \det (x\underline{I} - \underline{A}) \tag{1}$$

where $\underline{I}$ stands for the nxn unit matrix.

---

* For Parts I, II and IV: see [1], [2] and [3], respectively.

** Permanent address: "Ruder Bosković" Institute, YU-41001 Zagreb, Croatia, Yugoslavia.

The matching polynomial $\alpha(G) \equiv \alpha(G;x)$ is a purely combinatorial object defined [4] in terms of the coefficients $p(G,k)$, $k = 0,1,\ldots,[n/2]$. $p(G,k)$ denotes the number of ways in which k independent edges can be selected in G; by definition: $p(G,0) = 1$. Thus all $p(G,k)$ are natural numbers.

Both polynomials play a significant role in the chemical applications of graph theory [4].

By expanding the determinant (1) two kinds of contributions appear: the "acyclic" ones which are described by $p(G,k)$'s and the "cyclic" ones. Therefore, for graphs possessing no cycles $\alpha(G)$ and $\Phi(G)$ coincide. For all other graphs $\alpha(G)$ and $\Phi(G)$ are different. It would be appealing if $\alpha(G;x)$ could be expressed as the characteristic polynomial $\Phi(\underline{W};x)$ of some matrix $\underline{W}$:

$$\alpha(G;x) = \Phi(\underline{W};x) \equiv \det\,(x\underline{I} - \underline{W}) \quad . \tag{2}$$

If this is the case $\underline{W}$ defines the "acyclic" reference structure of a molecule described by graph G [5]. Since the roots of $\alpha(G;x)$ are real [6] the nxn matrix $\underline{W}$ has to be Hermitian ($\underline{W}^{\dagger} \equiv \underline{W}$).

The matrix $\underline{W}$ could be understood as a weight matrix related to G. We require that all zero elements of $\underline{A}(G)$ correspond to zero elements of $\underline{W}(G)$, i.e. the structure of $\underline{A}(G)$ and $\underline{W}(G)$ is the same.

By expanding the determinant (2) one immediately sees that all $p(G,k)$'s are expressed by some sums of particular k-linear products of $(W_{rs}W_{sr})$. In order to produce the correct weight function for any transposition we have to choose:

$$W_{rs}\,W_{sr} = 1 \tag{3}$$

for every non-zero element of $\underline{W}$.

By applying the Sachs theorem [4] to $\Phi(\underline{W};x) \equiv \det(x\underline{I} - \underline{W})$ one obtains the "acyclic" contributions which coincide with p(G,K)'s of $\alpha(G;x)$ as well as the "cyclic" contributions of the form: $W_{rs}W_{st}\ldots W_{uv}W_{vs}$ (where all r,s,t,..., u and v are different and the corresponding contribution $A_{rs}A_{st}\ldots A_{uv}A_{vs}$ is different from zero). Obviously, if every cyclic contribution equals zero eq. (2) is satisfied; such a solution is called a *trivial solution* of eq. (2). The question arises whether the trivial solution is compatible with the choice of any W_{rs}, r,s = 1,2,...,n.

The nature of the weights W_{rs} has not been specified up to now.

Let us consider W_{rs} as complex numbers:

$$W_{rs} = W^{*}_{sr} = A_{rs}\exp(i\Theta_{rs}) \qquad (4)$$

The trivial solution of eq. (2) is compatible with some choice of the parameters Θ_{rs} only for polycyclic graphs where no two cycles are condensed, in particular for monocyclic graphs [7]. For polycyclic condensed graphs the trivial solution is incompatible with any choice of the parameters Θ_{rs} [8].

However, for particular graphs [1,8,9] exhibiting symmetry a so called *collective solution* of eq. (2) can be found.

Bearing the above limitations in mind one could consider the use of more general numbers for representing W_{rs} than the complex numbers are.

Hamilton was the first to realize [10] that the complex field cannot be extended by adding just one more imaginary unit but can be extended to three such units, usually denoted by $\underline{i}$, $\underline{j}$ and $\underline{k}$, with the known non-commutative multiplication rules [2,10,11]. Further details on the algebra of quaternions are given, e.g. in our preceeding paper [2]. The notation used there will be used in the text.

Here and in the text that follows we search for the trivial solutions of eq. (2) with the matrix elements of $\underline{W}$ being *normalized quaternions*. We choose:

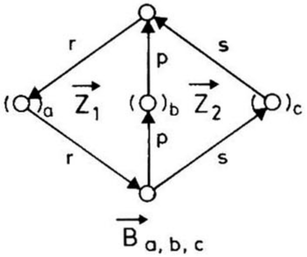
$$W_{rs} = A_{rs}(\cos \Theta_{rs} + \sin \Theta_{rs} \cdot \underline{v}_{rs}) \quad ,$$
$$W_{sr} = W^{*}_{rs} = A_{rs}(\cos \Theta_{rs} - \sin \Theta_{rs} \cdot \underline{v}_{rs}) \quad . \tag{5}$$

The above choice complies with eq. (2) and with the requirement that $\underline{W}$ has to be Hermitian. Moerover, the structure of $\underline{A}$ and $\underline{W}$ is the same for a given G.

In the previous paper [2] it was proved that the trivial solution of eq. (2) for (general, unsymmetrical) tricyclic peri-condensed graphs is compatible with different choices of quaternionic weights.

In the present paper we prove that also in the case of (general, unsymmetrical) bicyclic and tricyclic cata-condensed graphs there exist Θ'_{rs} and $\underline{v}_{rs}$'s compatible with the trivial solution of eq. (2).

Let us first consider the class $\mathcal{B}$ of bicyclic graphs. A typical representative of $\mathcal{B}$ is denoted by $B_{a,b,c}$ where a and c are natural numbers and b is a natural number or zero. The related weight matrix $\underline{W}$ can be represented by the directed weighted graph $\vec{B}_{a,b,c}$ and its counterpart $\overleftarrow{B}_{a,b,c}$; in the latter graph all arcs point in the directions opposite to those of $\vec{B}_{a,b,c}$. For reasons of simplicity only $\vec{B}_{a,b,c}$ is presented below. Let us further assume that all weights on the path belonging both to $\vec{Z}_1$ and $\vec{Z}_2$ are equal to some normalized quaternion: $p = \cos \Theta_p + \sin \Theta_p \cdot \underline{v}_p$, and that all related arcs in $\vec{B}_{a,b,c}$ form a directed path as is indicated below. The same convention is adopted also for the quaternionic weights in the outer paths of $\vec{Z}_1$ and $\vec{Z}_2$; these weights are denoted by: $r = \cos\Theta_r + \sin\Theta_r \cdot \underline{v}_r$ and $s = \cos\Theta_s + \sin\Theta_s \cdot \underline{v}_s$, respectively.



$\vec{Z}_3 = \vec{Z}_1 \cup \vec{Z}_2$

The trivial solution of eq. (2) requires that the cyclic contributions from $\vec{Z}_1$ (and $\overleftarrow{Z}_1$), $\vec{Z}_2$ (and $\overleftarrow{Z}_2$) and $\vec{Z}_3$ (and $\overleftarrow{Z}_3$) vanish. Therefore, eq. (2) implies:

$$\mathrm{Re}\{p^{b+1}\ r^{a+1}\} = 0 \quad , \qquad (6a)$$

$$\mathrm{Re}\{p^{b+1}\ (s^*)^{c+1}\} = 0 \quad , \qquad (6b)$$

$$\mathrm{Re}\{r^{a+1}\ s^{c+1}\} = 0 \quad . \qquad (6c)$$

One can check that for the following choice:

$$p^{b+1} = \underline{i} \quad , \quad r^{a+1} = \underline{j} \quad , \quad s^{c+1} = \underline{k} \qquad (7)$$

eqs. (6a) - (6c), i.e. eq. (2), are satisfied.

By using the following convenient property valid for the powers of quaternion [2,10,11]

$$q = \cos\Theta + \sin\Theta \cdot \underline{v} \quad , \quad q^n = \cos n\Theta + \sin n\Theta \cdot \underline{v} \qquad (8)$$

eq. (7) can be rewritten as:

$$p = \cos \frac{\pi}{2(b+1)} + \sin \frac{\pi}{2(b+1)} \cdot \underline{i} \quad , \tag{9a}$$

$$r = \cos \frac{\pi}{2(a+1)} + \sin \frac{\pi}{2(a+1)} \cdot \underline{j} \quad , \tag{9b}$$

$$s = \cos \frac{\pi}{2(c+1)} + \sin \frac{\pi}{2(c+1)} \cdot \underline{k} \quad , \tag{9c}$$

and these particular quaternionic weights are compatible with the trivial solution of eq. (2) in bicyclic graphs.

It has been shown [11,12] that the algebra of quaternions can be represented by means of the complex 2 x 2 matrices or the real 4 x 4 matrices. We adopt the latter representation and we represent four units of the algebra of quaternions by the following matrices:

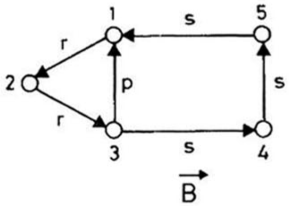
$$1 \rightarrow \underline{1} = \left[\begin{array}{cc|cc} 1 & 0 & \multicolumn{2}{c}{\underline{0}} \\ 0 & 1 & & \\ \hline \multicolumn{2}{c|}{\underline{0}} & 1 & 0 \\ & & 0 & 1 \end{array}\right] , \qquad \underline{i} \rightarrow \underline{I} = \left[\begin{array}{cc|cc} \multicolumn{2}{c|}{\underline{0}} & 1 & 0 \\ & & 0 & 1 \\ \hline -1 & 0 & \multicolumn{2}{c}{\underline{0}} \\ 0 & -1 & & \end{array}\right] ,$$

$$\underline{j} \rightarrow \underline{J} = \left[\begin{array}{cc|cc} 0 & 1 & \multicolumn{2}{c}{\underline{0}} \\ -1 & 0 & & \\ \hline \multicolumn{2}{c|}{\underline{0}} & 0 & -1 \\ & & 1 & 0 \end{array}\right] , \qquad \underline{k} \rightarrow \underline{K} = \left[\begin{array}{cc|cc} \multicolumn{2}{c|}{\underline{0}} & 0 & -1 \\ & & 1 & 0 \\ \hline 0 & -1 & \multicolumn{2}{c}{\underline{0}} \\ 1 & 0 & & \end{array}\right] . \tag{10}$$

By means of these matrices an arbitrary quaternion q can be represented by the corresponding 4 x 4 real matrix $\underline{Q}$. Therefore, instead of the original nxn matrix $\underline{W}$ of graph G with n vertices we could consider the 4n x 4n matrix $\underline{\mathcal{W}}$ which is obtained from $\underline{W}$ after the substitution: $q \rightarrow \underline{Q}$ and $1 \rightarrow \underline{1}$.

Therefore, once the Hermitian nxn weight matrix $\underline{W}$ compatible with the trivial solution of eq. (2) has been formed for a given G with n vertices, one generates by means of eq. (10) the related 4n x 4n real, symmetrical matrix $\underline{\mathcal{W}}$ which can then be diagonalized in a standard manner. The eigenvalues of $\underline{W}$, i.e. the roots of $\alpha(G;x)$ form the matching spectrum of G; the spectrum of $\underline{\mathcal{W}}$ contains four times the matching spectrum of G.

Let us illustrate the above findings by the example of the bicyclic graph $B \equiv B_{1,0,2}$. Its directed weighted graph $\vec{B}$ is depicted below together with the corresponding quaternionic weights.



According to eqs. (9a) - (9c) the trivial solution of eq. (2) for B is given by the following weights:

$$p = \underline{i} \quad , \quad r = \cos\frac{\pi}{4} + \sin\frac{\pi}{4} \cdot \underline{j} = \frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} \cdot \underline{j} \quad ,$$
$$s = \cos\frac{\pi}{6} + \sin\frac{\pi}{6} \cdot \underline{k} = \frac{\sqrt{3}}{2} + \frac{1}{2} \cdot \underline{k} \quad . \tag{11}$$

Accordingly the zeros ($x_1 = -x_5 = 2.17533$, $x_2 = -x_4 = 1.12603$, $x_3 = 0$) of $\alpha(B;x)$ are contained four times in the eigenvalues of the following weight matrix $\underline{\mathcal{W}}$:

$$\underline{W} = \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \left[\begin{array}{ccccc} \underline{O} & \underline{R} & \underline{P}^T & \underline{O} & \underline{S}^T \\ \underline{R}^T & \underline{O} & \underline{R} & \underline{O} & \underline{O} \\ \underline{P} & \underline{R}^T & \underline{O} & \underline{S} & \underline{O} \\ \underline{O} & \underline{O} & \underline{S}^T & \underline{O} & \underline{S} \\ \underline{S} & \underline{O} & \underline{O} & \underline{S}^T & \underline{O} \end{array}\right] \end{array} \qquad (12)$$

where according to eqs. (10) - (11) the matrix representatives $\underline{P}$, $\underline{R}$ and $\underline{S}$ of p, r and s, respectively, are given by:

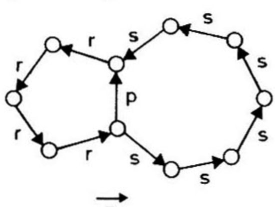
$$\underline{P} \equiv \underline{I} = \left[\begin{array}{cc|cc} \multicolumn{2}{c|}{\underline{O}} & 1 & 0 \\ & & 0 & 1 \\ \hline -1 & 0 & \multicolumn{2}{c}{\underline{O}} \\ 0 & -1 & & \end{array}\right] , \qquad \underline{R} = \left[\begin{array}{cc|cc} \sqrt{2}/2 & \sqrt{2}/2 & \multicolumn{2}{c}{\underline{O}} \\ -\sqrt{2}/2 & \sqrt{2}/2 & & \\ \hline \multicolumn{2}{c|}{\underline{O}} & \sqrt{2}/2 & -\sqrt{2}/2 \\ & & \sqrt{2}/2 & \sqrt{2}/2 \end{array}\right] \qquad (13)$$

$$\underline{S} = \left[\begin{array}{cc|cc} \sqrt{3}/2 & 0 & 0 & -1/2 \\ 0 & \sqrt{3}/2 & 1/2 & 0 \\ \hline 0 & -1/2 & \sqrt{3}/2 & 0 \\ 1/2 & 0 & 0 & \sqrt{3}/2 \end{array}\right]$$

and $\underline{P}^T$ denotes the transpose of the matrix $\underline{P}$.

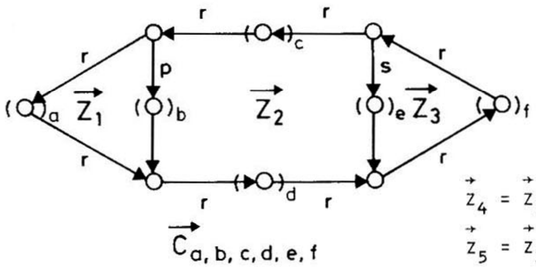
An example of a non-symmetric bicyclic graph meaningful in chemistry is provided by graph $B_{3,0,5}$ corresponding to azulene ($\vec{B}_{3,0,5}$) is shown below. In a similar manner as above we obtain

$$p = \underline{i} \ , \quad r = \cos\frac{\pi}{8} + \sin\frac{\pi}{8}\cdot\underline{j} \ , \quad s = \cos\frac{\pi}{12} + \sin\frac{\pi}{12}\cdot\underline{k} \ .$$



$\vec{B}_{3,0,5}$

Let us now consider class C of tricyclic cata-condensed graphs. A typical representative of C is denoted by $C_{a,b,c,d,e,f}$ where a and f are natural numbers and b, c, d and e are natural numbers and/or zero. All the conventions used previously for the bicyclic graphs are adopted here too. The directed weighted graph $\vec{C}_{a,b,c,d,e,f}$ related to $\underline{W}$ is depicted below where the quaternionic weights are indicated as well. It should be noted that in order to simplify the algebra we have chosen the same quaternionic weight v for all peripheric arcs in the graph depicted below.



$\vec{Z}_4 = \vec{Z}_1 \cup \vec{Z}_2$

$\vec{Z}_5 = \vec{Z}_2 \cup \vec{Z}_3$

$\vec{Z}_6 = \vec{Z}_1 \cup \vec{Z}_1 \cup \vec{Z}_3$

The trivial solution of eq. (2) requires that each of the cyclic contributions vanishes. Accordingly, eq. (2) gives rise to:

$$\mathrm{Re}\{r^{a+1}(p^*)^{b+1}\} = 0 \quad , \quad \mathrm{Re}\{r^{c+1}p^{b+1}r^{d+1}(s^*)^{e+1}\} = 0,$$

$$\mathrm{Re}\{r^{f+1}s^{e+1}\} = 0 \quad , \quad \mathrm{Re}\{r^{c+a+d+3}(s^*)^{e+1}\} = 0 \quad , \qquad (14)$$

$$\mathrm{Re}\{r^{d+f+c+3}p^{b+1}\} = 0 \quad , \quad \mathrm{Re}\{r^{a+c+d+f+4}\} = 0 \quad .$$

Let us choose:

$$p^{b+1} = \underline{i}, \quad \underline{s}^{e+1} = \underline{j} \quad . \tag{15}$$

Simple algebra then yields the following form of the weight r:

$$r = \cos \Theta_r + \sin \Theta_r \cdot \underline{k} \quad . \tag{16}$$

Eqs. (15) - (16) are compatible with eq. (14). Therefore, by using the convenient property (8) one obtains the following particular quaternionic weights of $\underline{W}$:

$$p = \cos \frac{\pi}{2(b+1)} + \sin \frac{\pi}{2(b+1)} \cdot \underline{i} \quad , \tag{17a}$$

$$s = \cos \frac{\pi}{2(e+1)} + \sin \frac{\pi}{2(e+1)} \cdot \underline{j} \quad , \tag{17b}$$

$$r = \cos \frac{\pi}{2(a+c+d+f+4)} + \sin \frac{\pi}{2(a+c+d+f+4)} \cdot \underline{k} \quad , \tag{17c}$$

which are compatible with the trivial solution of eq. (2) for the tricyclic cata-condensed graphs. If the four units of the algebra of quaternions in the above equations are represented by the appropriate real 4 x 4 matrices (10), the diagonalization of the related matrix $\underline{W}$ gives (four times) the matching spectrum of the tricyclic cata-condensed graph under consideration.

Similar findings apply also to tricyclic peri-condensed graphs. The matrix $\underline{W}$ exists for these graphs with the elements reported in the previous paper [2].

The use of quaternionic edge weights is no guarantee for finding a trivial solution for graphs with a large number of cycles. In such cases either collective solutions or a system of more general numbers for the edge weights must be used.

Acknowledgement. This work was supported in part by the National Science Foundation (Grant No. JFP-684). One of us (A.G.) thanks the Max-Planck-Gesellschaft for a grant.

REFERENCES

[1] A. Graovac and O.E. Polansky, MATCH, this issue.

[2] O.E. Polansky and A. Graovac, MATCH, this issue, preceeding paper.

[3] O.E. Polansky and A. Graovac, MATCH, this issue, following paper.

[4] For details on the use of graph theory in chemistry see: A. Graovac, I. Gutman, and N. Trinajstić, Topological Approach to the Chemistry of Conjugated Molecules, Springer-Verlag, Berlin 1977; N. Trinajstić, Chemical Graph Theory, Vols. 1-2, CRC Press, Boca Raton, Florida 1983; I. Gutman and O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin 1986.

[5] I. Gutman, M. Milun, and N. Trinajstić, MATCH 1 (1975) 171; J. Amer. Chem. Soc. 99 (1977) 1692; J. Aihara, J. Amer. Chem. Soc. 98 (1976) 2750.

[6] C.D. Godsil and I. Gutman, Z. Naturforsch. 34a (1979) 776; J. Graph Theory 5 (1981) 137.

[7] J. Aihara, Bull. Chem. Soc. Japan 52 (1979) 1529; L.J. Schaad, B.A. Hess, Jr., J.B. Nation, N. Trinajstić and I. Gutman, Croat. Chem. Acta 52 (1979) 233; A. Graovac, D. Kasum, and N. Trinajstić, Croat. Chem. Acta 54 (1981) 91.

[8] I. Gutman, A. Graovac, and B. Mohar, MATCH 13 (1982) 129.

[9] A. Graovac, Chem. Phys. Lett. 82 (1981) 248.

[10] W.R. Hamilton, Elements of Quaternions, Vols. 1-2, Chelsea, New York 1899, 1901; reprinted: 1969.

[11] S.L. Altman, Rotations, Quaternions, and Double Groups, Clarendon Press, Oxford 1986.

[12] L. Mirsky, An Introduction to Linear Algebra, Clarendon Press, Oxford 1955.