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

ON SOME GRAPHS WHOSE MATCHING POLYNOMIAL IS THE CHARACTERISTIC POLYNOMIAL OF A HERMITIAN MATRIX

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ABSTRACT

For a particular tetracyclic graph and for K_4 a weight matrix $\underline{W}$ is given, the characteristic polynomial of which coincides with the matching polynomial of the respective graphs. The entries of $\underline{W}$ are complex numbers.

In the chemical applications of graph theory a graph G is associated with a molecule in a prescribed manner [1]. Two polynomials play a significant role there: the characteristic polynomial $\phi(G;x)$ and the matching polynomial $\alpha(G;x)$ of G.

The characteristic polynomial is derived from the adjacency matrix. Any two vertices r and s in G are connected by an edge e(r,s) in G or they are not connected. The adjacency matrix $\underline{A} = \underline{A}(G)$ re-

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flects this basic information on G. Its matrix elements are defined as follows:

$$A_{rs} = A_{sr} = 1 \quad \text{if the edge } e(r,s) \text{ exists in G, and} \qquad A_{rs} = 0 \quad \text{otherwise} \tag{1}$$

$\underline{A}$ is an nxn symmetrical matrix where n stands for the number of vertices in G. Obviously, the eigenvalues of $\underline{A}$ are real numbers. They are related to the molecular orbital (MO) energies of a molecule described by G within some simple tight-binding Hamiltonian. The eigenvalues of $\underline{A}$ are the zeros of the characteristic polynomial which is defined by [1]

$$\Phi(G) = \Phi(G;x) = \det(x\underline{I} - \underline{A}) \tag{2}$$

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

The matching polynomial of G is defined by [2]

$$\alpha(G) = \alpha(G;x) = \sum_{k=0}^{n/2} (-1)^k \, p(G,k) \, x^{n-2k} \tag{3}$$

where p(G,k) denotes the number of ways in which $\underline{k}$ independent edges can be selected in G. Thus all p(G,k) are natural numbers; in addition: p(G,0) = 1 and p(G,1) = m, where m denotes the number of edges in G. The matching polynomial has found applications in chemistry: the reference energy of a conjugated molecule can be expressed in terms of the zeros of $\alpha(G;x)$ [3]; it also plays some role in statistical thermodynamics, for instance in calculations of the heats of adsorption, phase-transitions, etc. [4].

$\alpha(G)$ and $\Phi(G)$ generally differ; they coincide only for graphs possessing no cycles. It would be attractive if $\alpha(G)$ could be expressed in a manner analogous to eq. (2):

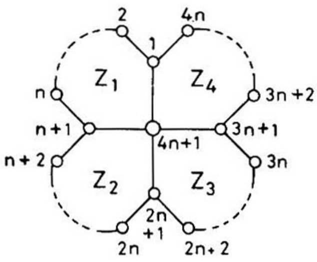
$$\alpha(G;x) = \Phi(\underline{W};x) = \det(x\underline{I} - \underline{W}) \tag{4}$$

where $\underline{W}$ stands for an nxn Hermitian matrix associated with some weighted digraph G^* of G and $\Phi(\underline{W};x)$ denotes the characteristic polynomial of that matrix. If this were the case, another proof of the reality of the zeros of $\alpha(G;x)$ follows immediately and, moreover, G^* may be interpreted in some way as the graph of the reference structure of a molecule. The existence of $\underline{W}$ (i.e. the search for $\underline{W}$ satisfying eq. (4)) was proved only for polycyclic graphs where no two cycles are condensed, in particular for monocyclic graphs [5], and in the case of condensed polycyclic graphs only for symmetrical bicyclic [6] and symmetrical peri-condensed tricyclic graphs [7]. As for an arbitrary (non-symmetrical) bicyclic graph no matrix $\underline{W}$ satisfying eq. (4) can be given explicitely it is easy to show that for graphs possessing more than two condensed cycles $\underline{W}$ cannot be generally given too [7].

However, for particular classes of polycyclic condensed graphs $\underline{W}$ can be found.

In the present note we consider the symmetrical tetracyclic peri-condensed graphs of class $\mathcal{B}$. Its typical representative B_n (with (4n+1) vertices) is depicted below. We prove that $\underline{W}$ exists for all graphs of class $\mathcal{B}$. In addition we shall prove that $\underline{W}$ exists also for the complete graphs K_3 and K_4.

In the following text we use in general the notations of Ref. [7].



(Bn)

$$Z_5 = Z_1 \cup Z_2$$
$$Z_6 = Z_2 \cup Z_3$$
$$Z_7 = Z_3 \cup Z_4$$
$$Z_8 = Z_4 \cup Z_1$$

$$Z_9 = Z_1 \cup Z_2 \cup Z_3$$
$$Z_{10} = Z_2 \cup Z_3 \cup Z_4$$
$$Z_{11} = Z_3 \cup Z_4 \cup Z_1$$
$$Z_{12} = Z_4 \cup Z_1 \cup Z_2$$

$$Z_{13} = Z_1 \cup Z_2 \cup Z_3 \cup Z_4 \setminus \{(4n + 1)\}$$

Let us replace the edges of G by pairs of oppositely directed arcs. If further a weight W_{rs} is associated with the arc starting at the vertex r and ending at the vertex s, a weighted digraph G^* of G is obtained. The weights W_{rs} define the weight matrix $\underline{W}(G^*)$ of G^*. $\underline{W}$ is related to the adjacency matrix $\underline{A}$ in such way that all zero elements of $\underline{A}$ correspond to zero elements in $\underline{W}$.

Expanding the determinant (4) one immediately sees that all p(G,k)'s are expressed by some sums of particular k-linear products of $(W_{rs}W_{sr})$. Bearing in mind that p(G,k)'s are natural numbers the choice

$$W_{rs}W_{sr} = 1 \tag{5}$$

represents the simplest way to meet the requirements for all non-zero elements of $\underline{W}$.

Note that the non-zero elements of the adjacency matrix also comply with the similar condition: $A_{rs}A_{sr} = 1$, simply because they equal 1. In order to obtain the different polynomials defined by eqs. (2) and (4), $\underline{A}$ and $\underline{W}$ should be different; in general, W_{rs} must be different from 1. In view of eq. (5) we choose:

$$W_{rs} = W^{*}_{sr} = A_{rs}\exp(i\Theta_{rs}) \tag{6}$$

Obviously: $\theta_{rs} = -\theta_{sr}$. The above choice reflects the fact that the structure of G and G* is the same as well as that $\underline{W}$ is Hermitian. Moreover, because of $W_{rs}W_{sr} = (A_{rs})^2 = 1$, one has:

$$\alpha(G^{*};x) = \alpha(G;x) \tag{7}$$

Let us consider a cycle Z in G of length $|Z|$. For reasons of simplicity we shall assume that vertices 1 and $|Z|$ and also r and r+1, r = 1,2,..., Z -1 are connected in Z; in addition: $|Z| > 2$. A cycle Z in G gives rise to two oppositely directed cycles in G*, the first one having the weight $\exp i(\Theta_{12}+\Theta_{23}+ \ldots + \Theta_{|Z|,1})$ and the second one having the weight $\exp i(\Theta_{1,|Z|} + \Theta_{|Z|,|Z|-1} + \ldots + \Theta_{2,1}) = \exp(-i(\Theta_{12} + \Theta_{23} + \ldots + \Theta_{|Z|,1}))$, i.e. the contribution of Z in G* equals 2t where:

$$t = \cos(\Theta_{12} + \Theta_{23} + \ldots + \Theta_{|Z|-1,|Z|} + \Theta_{|Z|,1}) \tag{8}$$

Obviously, the contribution of Z in G equals 2.

Bearing the above in mind and by applying the Sachs theorem [1] to the characteristic polynomial $\Phi(G;x)$ of G it has been shown recently [8] that $\Phi(G;x)$ is related to the matching polynomial of G in the following way:

$$\Phi(G) = \alpha(G) - 2\sum_{a}\alpha(G-Z_a) + 4\sum_{a<b}\alpha(G-Z_a-Z_b) - \\ - 8\sum_{a<b<c}\alpha(G-Z_a-Z_b-Z_c) + \ldots$$

where Z_a, a = 1,2,..., are the cycles of the graph G. Note that the second, third, etc. summations on the right-hand side go over pair-wise disjoint cycles.

Similarly, in view of (8) and by applying the Sachs theorem to $\Phi(\underline{W};x) = \det(x\underline{I}-\underline{W})$ [6] one obtains [7]:

$$\Phi(\underline{W}) = \alpha(G) - 2\sum_{a} t_a\, \alpha(G-Z_a) + 4\sum_{a<b} t_a t_b\, \alpha(G-Z_a-Z_b) - $$
$$- 8\sum_{a<b<c} t_a t_b t_c\, \alpha(G-Z_a-Z_b-Z_c) + \ldots$$

where t_a corresponding to the cycle Z_a is of the form (8).

Therefore, eq. (4) does agree with:

$$\sum_{a} t_a\, \alpha(G-Z_a) - 2\sum_{a<b} t_a t_b\, \alpha(G-Z_a-Z_b) + $$
$$+ 4\sum_{a<b<c} t_a t_b t_c\, \alpha(G-Z_a-Z_b-Z_c) - \ldots = 0 \qquad (9)$$

The matrix $\underline{W}$ can be given explicitely if a set of the parameters Θ_{rs} can be chosen such that eq. (9) holds.

Obviously, the choice: $t_a = 0$ for all a = 1,2,..., satisfies eq. (9). We call it a trivial solution of eq. (9). However, in the case of condensed polycyclic graphs no set of the parameters Θ_{rs} can be found which gives a *trivial solution*. Therefore, we continue to search for non-trivial solutions of eq. (9).

For the graphs of the class $\mathcal{B}$ there are no disjoint cycles possible and in this case eq. (9) reads as follows:

$$\sum_{j=1}^{13} t_j\, \alpha(G-Z_j;x) = 0 \qquad (10)$$

Let us note that the symmetry of B_n implies:

$$\alpha(G-Z_1) = \alpha(G-Z_2) = \alpha(G-Z_3) = \alpha(G-Z_4) = \alpha(P_{3n-1})$$

$$\alpha(G-Z_5) = \alpha(G-Z_6) = \alpha(G-Z_7) = \alpha(G-Z_8) = \alpha(P_{2n-1})$$

$$\alpha(G-Z_9) = \alpha(G-Z_{10}) = \alpha(G-Z_{11}) = \alpha(G-Z_{12}) = \alpha(P_{n-1})$$

$$\alpha(G-Z_{13}) = \alpha(P_1) = x$$

where P_ℓ stands for the path of the length ℓ. Because $\alpha(G-Z_1;x)$, $\alpha(G-Z_5;x)$, $\alpha(G-Z_9)$ and $\alpha(G-Z_{13})$ are polynomials in x of the mutually different orders, eq. (10) has to be partitioned into the following four conditions:

$$t_1 + t_2 + t_3 + t_4 = 0 \tag{11}$$

$$t_5 + t_6 + t_7 + t_8 = 0 \tag{12}$$

$$t_9 + t_{10} + t_{11} + t_{12} = 0 \tag{13}$$

$$t_{13} = 0 \tag{14}$$

Such a solution we call a *collective solution* of eq. (9).

Let us introduce the notation:

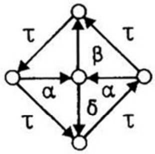
$$\begin{aligned}\tau &= \Theta_{12} + \Theta_{23} + \dots + \Theta_{n,n+1} = \\ &= \Theta_{n+1,n+2} + \dots + \Theta_{2n,2n+1} = \\ &= \Theta_{2n+1,2n+2} + \dots + \Theta_{3n,3n+1} = \\ &= \Theta_{3n+1,3n+2} + \dots + \Theta_{4n,1}\end{aligned}$$

$$\alpha = \Theta_{n+1,4n+1} = \Theta_{3n+1,4n+1}$$

$$\beta = \Theta_{4n+1,1}$$

$$\delta = \Theta_{4n+1,2n+1}$$

Note, $\exp(i\tau)$ is the weight associated with the sequence of arcs leading from 1 to n+1, leading from n+1 to 2n+1, etc. Whether eqs. (11) - (14) have solution in τ, α, β and δ doesn't depend on n and it is sufficient to consider B_1 instead of the whole class $\mathcal{B}$. A diagrammatic representation, (B_1^*), of the directed weighted graph B_1^* is depicted below. For reasons of simplicity for each edge in B_1 only one directed arc in B_1^* is presented; further, instead of the weights, $\exp(i\Theta_{rs})$, only the parameters Θ_{rs} are drawn besides the related arcs.



(B_1^*)

Eqs. (11) - (14) now read as follows:

$$\cos(\tau+(\alpha+\beta))+\cos(\tau-(\alpha+\beta))+\cos(\tau+(\alpha+\delta))+\cos(\tau-(\alpha+\delta)) = 0 \qquad (15)$$

$$2\cos(2\tau)+\cos(2\tau+(\beta-\delta))+\cos(2\tau-(\beta-\delta)) = 0 \qquad (16)$$

$$\cos(3\tau+(\alpha+\beta))+\cos(3\tau-(\alpha+\beta))+\cos(3\tau+(\alpha+\delta))+\cos(3\tau-(\alpha+\delta)) = 0 \qquad (17)$$

$$\cos(4\tau) = 0 \qquad (18)$$

The last equation yields:

$$\tau = (2j + 1)\pi/8, \quad j = 0,1,2,... \qquad (19)$$

By applying the well known identity:

$$\cos x + \cos y = 2 \cos(x+y)/2 \cos(x-y)/2 \qquad (20)$$

to the remaining equations one obtains:

$$\cos(\alpha+\beta) + \cos(\alpha+\delta) = 0 \qquad (21)$$

$$1 + \cos(\beta-\delta) = 0 \qquad (22)$$

where both eqs. (15) and (17) give rise to the same eq. (21). Eq. (22) yields:

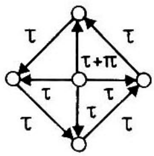
$$\beta = \delta + (2k+1)\pi, \quad k = 0,1,2,... \qquad (23)$$

and as a result eq. (21) is satisfied for any α and δ. Therefore, one has:

$$\alpha = \text{arbitrary}, \quad \delta = \text{arbitrary} \qquad (24)$$

The matrix $\underline{W}$ exists with the values of α, β, δ and τ being given by eqs. (19), (23) and (24).

A particular solution: $\alpha = \delta = \tau = \pi/8$, $\beta = \tau + \pi$ is shown below.

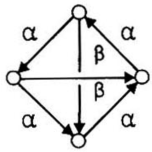


$\tau = \pi/8$

(B_1^*)

Note that the matrix $\underline{W}$ also exists with the same solution as given above if instead of B_n one considers graph obtained from B_n by replacing four edges incident to the vertex 4n+1 by the chains of arbitrary but equal lengths.

Let us now consider the complete graphs K_3 and K_4. The matrix $\underline{W}$ exists for K_3 since it is a monocyclic graph [3]. A directed weighted graph of K_4 for a particular choice of Θ_{rs}-parameters is shown below.

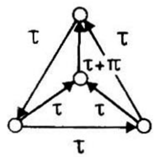


(K_4^*)

Simple algebra leads to the conclusion that the matrix $\underline{W}(K_4^*)$ exists for:

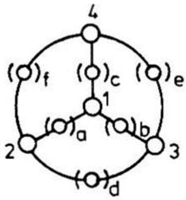
$$\alpha = (2j+1)\pi/8, \ \beta = (2k+1)\pi/2, \ j,k = 0,1,2,...$$

Another choice of the parameters Θ_{rs} for K_4 is obtained if it is represented as a planar tricyclic peri-condensed graph. The corresponding directed weighted graph is depicted below.



The matrix $\underline{W}$ exists for: $\tau = (2j+1)\pi/4$, $j = 0,1,2,...$ or for: $\tau = (6k\underline{+}1)\pi/6$, $k = 0,1,2,...$. (It is interesting to compare the above graph with the graph B_1^*: for both of them all parameters Θ_{rs} equal τ except one which equals $\tau + \pi$; however, τ has not the same value for both graphs.

Let G be a homeomorph of K_4 obtained by the subdivision of the edges of K_4 by appropriate numbers a,b,c,... of vertices as depicted schematically below:



$Z_1 = (1,\ldots,2,\ldots,3,\ldots,1)$

$Z_2 = (1,\ldots,3,\ldots,4,\ldots,1)$

$Z_3 = (1,\ldots,4,\ldots,2,\ldots,1)$

$Z_4 = (2,\ldots,3,\ldots,4,\ldots,2)$

$Z_5 = (1,\ldots,2,\ldots,3,\ldots,4,\ldots,1)$

$Z_6 = (1,\ldots,3,\ldots,4,\ldots,2,\ldots,1)$

$Z_7 = (1,\ldots,4,\ldots,2,\ldots,3,\ldots,1)$

The method of collective solution applied above requires the following equalities

$$\alpha(G-Z_1) = \alpha(G-Z_2) = \alpha(G-Z_3) = \alpha(G-Z_4) \quad , \qquad (25)$$

$$\alpha(G-Z_5) = \alpha(G-Z_6) = \alpha(G-Z_7) \quad . \qquad (26)$$

As can be shown easily these equalities hold only in case of

$$a = b = c = d = e = f \quad .$$

This means: the results obtained above for K_4 can be applied only to those tricyclic graphs with 6a+4 vertices which exhibit the same high symmetry as K_4 [9]. The conservation of the high symmetry seems to be a characteristic of the method of the collective solution.

Thus, one would conjecture that the symmetry requirements for the homeomorphs of K_4 might be reduced when the respective collections of the 3- and/or 4-membered cycles are partitioned into smaller ones. Such an attempt has already been reported in [7] where the requirement (25) is reduced to

$$\alpha(G-Z_1) = \alpha(G-Z_2) = \alpha(G-Z_3) \qquad (27)$$

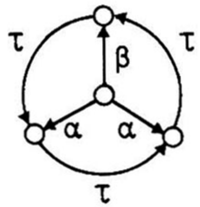
allowing one to apply the results to homeomorphs of K_4 with

$$a = b = c \quad \text{and} \quad d = e = f \quad .$$

Below we give some other weights for K_4 which require only the equalities (26). Unfortunately, this leads again to

$$a = b = c \quad \text{and} \quad d = e = f \quad .$$

Thus, a further reduction of the symmetry of the homeomorphs of K_4 demands a partitioning of the collection of the 4-membered cycles, but could not be achieved.



α = arbitrary

$\beta = \alpha + \pi$

$\tau = \frac{\pi}{2}$

In the subsequent paper [10] we present a trivial solution for K_4 obtained by means of quaternionic weights; the trivial solution for K_4 may be applied to any homeomorph of K_4.

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