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UNIQUENESS OF THE MATCHING POLYNOMIAL

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Abstract

If uv is an edge of a graph G, connecting the vertices u and v, and if $G_1 \cup G_2$ is the graph composed of two disconnected components G_1 and G_2, then the general nontrivial solution of the recurrence relations

$$I(G) = I(G - uv) + I(G - u - v) \qquad \& \qquad I(G_1 \cup G_2) = I(G_1) \cdot I(G_2)$$

is the matching polynomial $\alpha^+(G) = \sum_{k \geq 0} m(G,k)\, \lambda^{|G|-2k}$, where $|G|$ is the number of vertices of the graph G, and $m(G,k)$ the number of its k-matchings.

INTRODUCTION

In this paper we are concerned with simple graphs, that is graphs possessing neither multiple or directed or weighted edges, nor self–loops. Let G denote such a graph and $|G|$ be the number of its vertices.

The Kekulé structure count $K = K(G)$ and the Hosoya topological index $Z = Z(G)$ play a significant role in chemical graph theory. Details on K can be found in the book [1], the references cited therein, as well as in some recent papers [2–7]. Details on Z can be found in the book [8], review [9], the references cited therein, as well as in some recent papers [10–14].

A collection of k independent (i. e., mutually non-touching) edges in a graph is said to be a k-matching. The number of k-matchings of a graph G is denoted by $m(G,k)$. By definition, $m(G,0) = 1$ and $m(G,1) =$ the number of edges of G. The matching polynomial (earlier also known as the "acyclic polynomial" [15]) is a counting polynomial whose coefficients are the numbers $m(G,k)$. It is usually (but not always [16–18]) defined as

$$\alpha(G\,,\,\lambda) = \sum_{k\geq 0} (-1)^k\, m(G,k)\, \lambda^{|G|-2k}$$

in which case it has the remarkable property that, for trees, it coincides with the characteristic polynomial. Details on the matching polynomial and an exhaustive bibliography can be found in the book [19] and elsewhere [20–23]. In this paper we need a slightly modified form of the matching polynomial, namely

$$\alpha^+(G\,,\,\lambda) = \sum_{k\geq 0} m(G,k)\, \lambda^{|G|-2k}\ .$$

As easily seen, $\alpha^+(G\,,\,\lambda) = i^{-|G|}\, \alpha(G\,,\,i\,x)$, where $i = \sqrt{-1}$.

Two elementary properties of the α^+-polynomial are

$$\alpha^+(G\,,\,0) = K(G) \qquad \text{and} \qquad \alpha^+(G\,,\,1) = Z(G) \tag{1}$$

which are based on the fact that $K(G)$ is the number of perfect matchings of the graph G, whereas $Z(G)$ is the total number of matchings of the same graph. A less obvious property is that if the equation $\alpha^+(G\,,\,\lambda) = 0$ has a real–valued solution, then this solution is equal to zero. Furthermore, if $K(G) > 0$, then the equation $\alpha^+(G\,,\,\lambda) = 0$ has no real–valued solutions.

Consider an edge uv of a graph G, which connects the vertices u and v. Denote by $G - uv$ the graph obtained from G by deleting the edge uv. Denote by $G - u - v$ the graph obtained from G by deleting the vertices u and v and all edges incident to u and v. Then, of course, $|G - uv| = |G|$ and $|G - u - v| = |G| - 2$.

If u and v are the only vertices of G, then $G - u - v$ will have no vertices at all. This graph (or "graph") will be denoted by $\emptyset$.

As well and long known [2], the Kekulé structure count satisfies the relation

$$K(G) = K(G - uv) + K(G - u - v) \tag{2}$$

where uv may be any edge of G. Formula (2) is valid for any graph G, assuming that $K(\emptyset) = 1$.

If the graph G consists of two disconnected components G_1 and G_2 (which themselves may be disconnected), then we write $G = G_1 \cup G_2$. In this case,

$$K(G) = K(G_1) \cdot K(G_2)\ . \tag{3}$$

Fully analogous relations hold for the Hosoya index [8], namely:

$$Z(G) = Z(G - uv) + Z(G - u - v) \tag{4}$$

$$Z(G_1 \cup G_2) = Z(G_1) \cdot Z(G_2) \tag{5}$$

and also for the matching polynomial [19]:

$$\alpha(G\,,\,\lambda) = \alpha(G - uv\,,\,\lambda) - \alpha(G - u - v\,,\,\lambda)$$

$$\alpha(G_1 \cup G_2\,,\,\lambda) = \alpha(G_1\,,\,\lambda) \cdot \alpha(G_2\,,\,\lambda)$$

which in the case of α^+ becomes

$$\alpha^+(G\,,\,\lambda) = \alpha^+(G - uv\,,\,\lambda) + \alpha^+(G - u - v\,,\,\lambda) \tag{6}$$

$$\alpha^+(G_1 \cup G_2\,,\,\lambda) = \alpha^+(G_1\,,\,\lambda) \cdot \alpha^+(G_2\,,\,\lambda)\ . \tag{7}$$

In view of Eqs. (2)–(7), we may consider K, Z, and α^+ as three particular solutions of the following system of recurrence relations

$$\left.\begin{array}{ll} I(G) = I(G-uv) + I(G-u-v) & (8) \\ I(G_1 \cup G_2) = I(G_1) \cdot I(G_2) & (9) \end{array}\right\} \qquad (\mathbf{A})$$

where I stands for some graph invariant.

In what follows we demonstrate that α^+ is the the general solution of $(\mathbf{A})$ and that there are no solutions other than those of the form $\alpha^+(G\,,\,\lambda)$ with λ being either an indeterminate or a real– or complex–valued number.

SOLVING THE RECURRENCE RELATIONS (A)

We may ask whether $(\mathbf{A})$ has any solution other that $\alpha^+(G\,,\,\lambda)$, which – of course – includes all special cases of $\alpha^+(G\,,\,\lambda)$, such as K and Z, cf. Eq. (1).

There, indeed, exists such a solution: $I(G) \equiv 0$ for all graphs G. This we consider as the trivial solution, and it is of no interest to us. Thus, we will require that for at least some graph G, the invariant $I(G)$ is non-zero.

As usual, P_n denotes the path with n vertices.

When seeking for solutions of $(\mathbf{A})$ it is reasonable to start with graphs with as few vertices as possible. Thus we start with the single-vertex graph P_1 and the connected two-vertex graph P_2. (The two-vertex graph must be connected, since otherwise its I-value would simply be equal to $I(P_1)^2$.)

Let thus choose $I(P_1) = X$ and $I(P_2) = Y$.

Consider P_3 and apply (8) to any of its two edges. Because $P_3 - uv = P_2 \cup P_1$ and $P_3 - u - v = P_1$, in view of (9) we get:

$$I(P_3) = I(P_2) \cdot I(P_1) + I(P_1) = X\,(Y+1)\ .$$

Consider now P_4 and apply (8) to one of its terminal edges. Then $P_4 - uv = P_3 \cup P_1$ and $P_4 - u - v = P_2$, resulting in

$$I(P_4) = I(P_3) \cdot I(P_1) + I(P_2) = X^2\,(Y+1) + Y\ .$$

If, however, we apply (8) to the central edge of P_4, then $P_4 - uv = P_2 \cup P_2$ and $P_4 - u - v = P_1 \cup P_1$, resulting in

$$I(P_4) = I(P_2) \cdot I(P_2) + I(P_1) \cdot I(P_1) = Y^2 + X^2 \ .$$

Because the value of the invariant I must not depend on the choice of the edge to which we apply (8), it must be

$$X^2\,(Y+1) + Y = Y^2 + X^2$$

i. e.,

$$Y\,(X^2 - Y - 1) = 0 \ .$$

We thus have two options: $Y = 0$ and $Y = X^2 + 1$.

It is not difficult to see that the choice $Y = X^2 + 1$ produces the matching polynomial, since for $\alpha^+(P_1\,,\,\lambda) = \lambda \equiv X$ and $\alpha^+(P_2\,,\,\lambda) = \lambda^2 + 1 \equiv X^2 + 1$.

Thus, if the system (**A**) has any other nontrivial solution, it must be compatible with the choice $Y = 0$. If so, then $I(P_1) = X$, $I(P_2) = 0$, $I(P_3) = X$, $I(P_4) = X^2$. Based on these I-values we compute $I(P_5)$.

Applying (8) to the terminal edge of P_5 we get

$$I(P_5) = I(P_4 \cup P_1) + I(P_3) = X^2 \cdot X + X = X\,(X^2 + 1) \ .$$

Application of (8) to a non-terminal edge yields

$$I(P_5) = I(P_3 \cup P_2) + I(P_2 \cup P_1) = X \cdot 0 + 0 \cdot X = 0$$

which is consistent with the previous result only if either $X = 0$ or $X^2 + 1 = 0$.

The first of these two options, namely $X = Y = 0$ leads to the trivial solution of (**A**). Remains $X^2 + 1 = 0$ & $Y = 0$. This, however, is just the earlier obtained solution $Y = X^2 + 1$ for a particular value of the parameter X, i. e., $X = \pm i$, where $i = \sqrt{-1}$. Hence, this latter option leads to $\alpha^+(G\,,\,\pm i)$.

Although the above arguments are sufficient to demonstrate our claim, we may examine also the following starting point: $I(P_1) = X$ & $I(\emptyset) = Y$. If so, then using the same way of reasoning we get

$$I(P_2) = X^2 + Y \qquad ; \qquad I(P_3) = X^3 + X\,(Y+1)$$

$$I(P_4) = X^4 + X^2\,(Y+2) + Y \qquad \text{and} \qquad I(P_4) = X^4 + X^2\,(2Y+1) + Y^2\,.$$

Equating the right–hand sides of the latter two expressions we get

$$(Y-1)(X^2+Y) = 0$$

the solutions of which are $Y=1$ and $Y=-X^2$.

The first solution, $Y=1$, gives $I(P_2) = X^2+1$, $I(P_3) = X^3+2X$, $I(P_4) = X^4+3\,X^2+1$ and thus leads to the α^+-polynomial.

Choosing $Y=-X^2$ we obtain $I(P_2)=0$, $I(P_3)=X$, $I(P_4)=X^2$, whereas in the case of P_5 both

$$I(P_5) = I(P_1)\cdot I(P_4) + I(P_3) = X^3 + X$$

and

$$I(P_5) = I(P_2)\cdot I(P_3) + I(P_1)\cdot I(P_2) = 0$$

must hold, implying that either $X=0$ or $X^2+1=0$.

If $X=0$, then also $Y=-X^2=0$ are we arrive at the trivial solution.

If $X^2+1=0$, then $Y=-X^2=1$ and, as before, we arrive at the solution $\alpha^+(G\,,\,\pm i)$.

* * * * *

We thus have determined all graph invariants (those of interest in chemical graph theory, those that may one day become interesting, and those that never will be) that conform to the recurrence relations of the type (**A**). Our main result may be formulated as follows:

Theorem. The system of recurrence relations (**A**) has a trivial solution: $I(G)\equiv 0$ for all graphs G. The only nontrivial solution of (**A**) is of the form $\alpha^+(G\,,\,\lambda)$ where λ may assume any real or complex value.

References

[1] S. J. Cyvin, I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, Springer–Verlag, Berlin, 1988.

[2] I. Gutman, D. Vukičević, A. Graovac, M. Randić, Algebraic Kekulé structures of benzenoid hydrocarbons, *J. Chem. Inf. Comput. Sci.* **44** (2004) 296–299.

[3] M. Randić, Algebraic Kekulé formulas for benzenoid hydrocarbons, *J. Chem. Inf. Comput. Sci.* **44** (2004) 365–372.

[4] T. Morikawa, D. J. Klein, Quantification of π-electron capacity of Kekuléan substructures in benzenoid hydrocarbons, *Polyc. Arom. Comp.* **25** (2005) 129–140.

[5] A. Vesel, Characterization of resonance graphs of catacondensed hexagonal graphs, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 195–208.

[6] M. Lin, X. Guo, Ordering catacondensed hexagonal systems with small numbers of Kekulé structures, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 403–418.

[7] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[8] H. Hosoya, The topological index Z before and after 1971, *Internet Electr. J. Mol. Design* **1** (2002) 428–442.

[9] I. Gutman, B. Furtula, D. Vidović, H. Hosoya, A concealed property of the topological index Z , *Bull. Chem. Soc. Jpn.* **77** (2004) 491–496.

[10] X. Li, H. Zhao, Trees with the first smallest and largest generalized topological indices, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 57–62.

[11] B. Zhou, I. Gutman, Estimating the modified Hosoya index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 183–192.

[12] L. Ye, R. S. Chen, Ordering of trees with given bipartition by their energies and Hosoya indices, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 193–208.

[13] I. Gutman, S. Radenković, B. Furtula, H. Hosoya, Some properties of the topological bond order, *Chem. Phys. Lett.* **407** (2005) 73–77.

[14] I. Gutman, The acyclic polynomial of a graph, *Publ. Inst. Math. (Beograd)* **22** (1977) 63–69.

[15] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* **44** (1971) 2332–2339.

[16] E. J. Farrell, An introduction to matching polynomials, *J. Comb. Theory* **B 27** (1979) 75–86.

[17] I. Gutman, Some relations for the independence and matching polynomials and their chemical applications, *Bull. Acad. Serbe Sci. Arts* **105** (1992) 39–49.

[18] D. M. Cvetković, M. Doob, I. Gutman, A. Torgašev, *Recent Results in the Theory of Graph Spectra*, North–Holland, Amsterdam, 1988.

[19] C. D. Godsil, I. Gutman, On the theory of the matching polynomial, *J. Graph Theory* **5** (1981) 137–144.

[20] M. Randić, A route to acyclic (matching) polynomial, in: M. F. Capobianco, M. Guan, D. F. Hsu, F. Tian (Eds.), *Graph Theory and Its Applications: East and West*, New York Acad. Sci., New York, 1989, pp. 458–465.

[21] V. R. Rosenfeld, I. Gutman, A novel approach to graph polynomials, *MATCH Commun. Math. Chem.* **24** (1989) 191–199.

[22] G. G. Cash, W. C. Herndon, Novel approaches to exact coefficients of acyclic polynomials, *MATCH Commun. Math. Comput. Chem.* **40** (1999) 273–278.