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SOME ANALYTICAL PROPERTIES OF THE INDEPENDENCE AND MATCHING POLYNOMIALS

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Abstract: The first derivative of the independence polynomial of a graph is expressed as a sum of independence polynomials of its certain subgraphs. Analogous results are obtained also for the matching polynomials. This makes possible to unify and rationalize a number a previously known results for these graph polynomials and to gain a deeper insight into their combinatorial and analytical properties. A detailed outline of the physico-chemical applications of these polynomials is given in the Introduction.

INTRODUCTION

In this paper we are concerned with graph polynomials whose coefficients are the numbers $n(G,k)$ and $m(G,k)$.

Definition 1. The number of ways in which k, $k \geq 2$, independent (i.e. mutually nonadjacent) vertices can be selected in a graph G is denoted by $n(G,k)$. In addition to this, $n(G,0) = 1$ and $n(G,1)$ = number of vertices of the graph G.

Definition 2. The number of ways in which k, $k \geq 2$, independent (i.e. mutually nonincident) edges can be selected in a graph G is denoted by m(G,k). In addition to this, m(G,0) = 1 and m(G,1) = number of edges of the graph G.

The **independence polynomial** of the graph G is then defined as

$$\omega^{*}(G) = \omega^{*}(G,\ x) = \sum_{k\geq 0} n(G,k)\ x^{k} \quad . \qquad (1\ a)$$

This object seems to be first examined by Motoyama and Hosoya in 1977 and named "*king polynomial*" [1]. They, however, defined it for (square) lattices rather than for general graphs. The appropriate graph-theoretical reformulation of this concept was given by Balasubramanian and Ramaraj [2] who used the name "*color polynomial*". In the meantime the present author independently introduced ω^{*} within an algebraic approach to Clar's aromatic sextet theory [3]; somewhat later similar ideas were put forward by Herndon and Hosoya [4]. A systematic study of the mathematical properties of the independence polynomial was undertaken by Gutman and Harary [5] and quite recently by Hoede and Li [6].

In addition to its application in the Clar aromatic sextet theory [3,7], the independence polynomial is also worth studying because of its relation to the partition function for the magnetic properties of transition metal crystals [1,8], its role in the kinetics of adsorption of diatomic molecules on metal surfaces [1,9] and its usgae in the modeling of some other physico-chemical phenomena [1,2].

The so-called **matching polynomial** has a somewhat unusual history [10]. In 1971 Hosoya put forward his topological index Z [11]. For this purpose he used an auxiliary "*Z-counting polynomial*":

$$\alpha^{*}(G) = \alpha^{*}(G,\ x) = \sum_{k\geq 0} m(G,k)\ x^{k} \quad . \qquad (2\ a)$$

Another object of the same kind, namely

$$\alpha(G) = \alpha(G, x) = \sum_{k\geq 0} (-1)^k m(G,k) x^{n-2k} \qquad (2\ b)$$

plays a distinguished role in the so-called monomer-dimer theory of statistical physics and was studied in some detail especially by Heilmann and Lieb [12]. Somewhat later α was rediscovered within a theory of resonance energy [13,14] and was named "*acyclic*" [13] and "*reference*" [14] polynomial. The name matching polynomial was first utilized by Farrell [15] who independently arrived at it within a combinatorial context. The theory of the matching polynomial was eventually extensively elaborated [10,16,17] and a large number of its remarkable mathematical properties were discovered.

Whereas the quantities ω^* and α^*, defined via eqs. (1a) and (2a), are fully analogous, there is no independence-polynomial counterpart of α, eq. (2b). As we demonstrate in the subsequent sections, the pertinent form of such an independence polynomial seems to be

$$\omega(G) = \omega(G, x) = \sum_{k\geq 0} (-1)^k n(G,k) x^{n-k} \quad . \qquad (1\ b)$$

In this section we briefly outlined the main applications of the matching and independence polynomials in various fields of theoretical physics, theoretical chemistry and physical chemistry. These numerous applications suggest that the two polynomials might have interesting and non-trivial mathematical properties, and that their study is justified from the point of view of natural sciences and mathematical chemistry in particular. Indeed, many such studies have already been undertaken and quite a few intriguing results have been obtained (see, for instance, [6,10,17,18]). Nevertheless, analytical properties of the matching and independence polynomials (i.e. propereties related to their derivatives and integrals) have so far attracted little attention of researchers. The present paper is aimed to partially fill this gap and, hopefully, to initiate further investigations along the same line.

THE FIRST DERIVATIVE OF THE MATCHING AND INDEPENDENCE POLYNOMIALS

In [19] a result for the matching polynomial was reported which we restate in the form of

Theorem 1. The first derivative of the matching polynomial α, defined via eq. (2 b), conforms to the identity

$$(d/dx)\ \alpha(G) = \sum_{v} \alpha(G-v) \tag{3}$$

where G-v denotes the subgraph obtained by deleting the vertex v from the graph G, and where the summation goes over all vertices of G.

The vertex-deleted subgraph G-v is often called an Ulam subgraph [19]. Recall also that relations analogous to (3) hold in the case of the characteristic [17,20,21] as well as the μ-polynomial [22].

Similar, but not fully analogous, relations hold also for the polynomials α^{*}, ω and ω^{*}. We state them in the following three theorems. The formal demonstration of the validity of Theorems 2-4 as well as a novel proof of Theorem 1, completely different from the reasoning employed in [19], has been published elsewhere [23].

Theorem 2. The first derivative of the matching polynomial α^{*}, defined via eq. (2a), conforms fo the identity

$$(d/dx)\ \alpha^{*}(G) = \sum_{e(uv)} \alpha^{*}(G-u-v) \tag{4}$$

where e(uv) denotes an edge of the graph G whose endpoints are u and v, and where the summation goes over all edges of the graph G.

Theorem 3. The first derivative of the independence polynomial ω, defined via eq. (1b), conforms to the identity

$$(d/dx)\ \omega(G) = \sum_{v} \omega(G-v) \tag{5}$$

where the notation is the same as in Theorem 1.

Theorem 4. The first derivative of the independence polynomial ω^*, defined via eq. (1a), conforms to the identity

$$(d/dx)\ \omega^*(G) = \sum_{v} \omega^*(G-N_v) \tag{6}$$

where N_v is the set containing the vertex v and all its first neighbors, and where the summation goes over all vertices of the graph G.

DISCUSSION

A noteworthy feature of the above four theorems is the fact that the forms of eqs. (3) and (5) are fully analogous. A simple analysis reveals that this analogy is achieved by choosing the form of $\omega(G)$ as given in eq. (1b). It is easy to see that any other "independence polynomial" defined as

$$\omega_{gen}(G) = \sum_{k \geq 0} c_k\ n(G,k)\ x^{n-k}$$

where c_0, c_1, c_2,... are arbitrary constants, would obey the first-derivative formula (5), namely:

$$(d/dx)\ \omega_{gen}(G) = \sum_{v} \omega_{gen}(G-v)\quad . \tag{7}$$

Thus the choice (1b) which we have proposed is not the only possible one. Other forms of the ω-polynomial are conceivable. What, however, is necessary and unavoidable for a well-defined independence polynomial is that the coefficient of x^{n-k} is chosen to be proportional to n(G,k). If this is not the case, then no result analogous to Theorem 3 can exist.

The above conclusion can be rephrased in the following manner: The crucial condition for the validity of formula (5) is that n(G,k) is proportional to the coefficient of x^{n-pk}, $p = 1$. Similarly, eq. (3) holds because m(G,k) is the coefficient of x^{n-pk}, $p = 2$. This observation is readily generalized: The form of a graph polynomial based on the selection of independent fragments, each involving p vertices, has to be defined as

$$\zeta(G) = \sum_{k \geq 0} c_k \, i(G,k) \, x^{n-pk} \qquad (8\ b)$$

where i(G,k) is the number of ways in which k such independent fragments can be chosen and c_0, c_1, c_2,... are constants. In that case the first derivative of the polynomial $\zeta(G)$ conforms to the Ulam-subgraph expansion

$$(d/dx)\ \zeta(G) = \sum_{v} \zeta(G-v) \quad .$$

The above formula represents a generalization of both eqs. (3), (5) and (7). With regard to this, the expression (8b) may be considered as a recipe for defining novel combinatorial graph polynomials with convenient analytical properties.

SOME COROLLARIES OF THE THEOREMS 1-4

In this section we point out a few corollaries of Theorems 1-4. Some of them have been reported also in ref.[23], where more details on their proofs can be found.

It is remarkable that the two first-derivative formulas (3) and (4) have quite different forms. This difference is best seen from the below two corollaries of the Theorems 1 and 2, respectively:

Corollary 1.1.

$$\sum_{e(uv)} \alpha(G-u-v) = \frac{1}{2}\, x\, (d/dx)\, \alpha(G) - \frac{n}{2}\, \alpha(G) \quad .$$

Corollary 2.1.

$$\sum_{v} \alpha^{*}(G-v) = -2\, x\, (d/dx)\, \alpha^{*}(G) + n\, \alpha^{*}(G) \quad .$$

The ω^{*}-counterpart of Corollary 2.1 reads as follows.

Corollary 4.1.

$$\sum_{v} \omega^{*}(G-v) = -x\, (d/dx)\, \omega^{*}(G) + n\, \omega^{*}(G) \quad .$$

Comparing Corollaries 2.1 and 4.1 it is easy to see that for the graph polynomial ζ^{*}, defined as

$$\zeta^{*}(G) = \sum_{k\geq 0} i(G,k)\, x^{k} \qquad (8\ a)$$

will satisfy the relation

$$\sum_{v} \zeta^{*}(G-v) = -p\, x\, (d/dx)\, \zeta^{*}(G) + n\, \zeta^{*}(G)$$

where the same notation as in eq. (8b) is used.

Unfortunately, it is not possible to find a formula which would be complementary to Corollary 1.1 and which would relate the first derivative of $\omega(G)$ with the sum of $\omega(G-N_v)$-terms. Namely, ω satisfies the relation

$$\omega(G) = x\ \omega(G-v) - x^{d(v)}\ \omega(G-N_v) \qquad (9)$$

where d(v) denotes the degree of the vertex v. As a consequence of eq. (9), the sum of the $\omega(G-N_v)$-terms depends both on the Ulam-subgraphs and on the respective vertex degrees.

Corollary 3.1a.

$$\sum_v \omega(G-N_v) = x \sum_v x^{-d(v)}\ \omega(G-v) - \omega(G) \sum_v x^{-d(v)} \quad .$$

This is a rather complicated structure-dependence, indeed. On the other hand, the above result can be expressed in a somewhat simpler manner:

Corollary 3.1b.

$$\sum_v x^{d(v)}\ \omega(G-N_v) = x\ (d/dx)\ \omega(G) - n\ \omega(G) \quad .$$

Corollary 3.2. If G is a regular graph of degree r, then

$$\sum_v \omega(G-N_v) = x^{-r}\ [x\ (d/dx)\ \omega(G) - n\ \omega(G)] \quad .$$

Suppose that H is a symmetric n-vertex graph whose all Ulam subgraphs H-v are mutually isomorphic. Then some of the above stated results are significantly simplified.

Corollary 1.2. Let ζ be a graph polynomial of the type (8). In particular, ζ may stand for α or ω. Then for a symmetric graph H

$$(d/dx)\ \zeta(H) = n\ \zeta(H-v) \quad .$$

Corollary 2.2. For a symmetric graph H,

$$(d/dx)\ \alpha^*(H) = \frac{1}{2}\,\frac{n}{x}\,[\alpha^*(H) - \alpha^*(H-v)] \quad .$$

Corollary 4.2. For a symmetric graph H,

$$(d/dx)\ \omega^*(H) = \frac{n}{x}\,[\omega^*(H) - \omega^*(H-v)] \quad .$$

Comparing Corollaries 2.2 and 4.2 it is clear that they are special cases of the formula

$$(d/dx)\ \zeta^*(H) = \frac{1}{p}\,\frac{n}{x}\,[\omega^*(H) - \omega^*(H-v)]$$

where the polynomial ζ^* is defined via eq. (8 a).

In order to complete the summation formulas deduced in this paper we report expressions [23] for the sums of the independence polynomials of the subgraphs G-u-v where u and v are adjacent vertices of the graph G and where e(u,v) stands for the edge connecting u and v.

Corollary 3.3. For a graph G with m edges,

$$\sum_{e(u,v)} \omega(G-u-v) = x^{-2}\,[x \sum_{v} d(v)\ \omega(G-v) - m\ \omega(G)] \quad .$$

Corollary 3.4. If G is a regular graph of degree r, then

$$\sum_{e(u,v)} \omega(G-u-v) = x^{-2}\,[r\ x\ (d/dx)\ \omega(G) - m\ \omega(G)] \quad .$$

Recall that for such a graph $m = \frac{1}{2}\,n\,r$.

Corollary 4.3. For a graph G with m edges,

$$\sum_{e(u,v)} \omega^*(G-u-v) = \sum_{v} d(v)\ \omega^*(G-v) - m\ \omega^*(G) \quad .$$

Corollary 4.4. If G is a regular graph of degree r, then

$$\sum_{e(u,v)} \omega^{*}(G-u-v) = -r\ x\ (d/dx)\ \omega^{*}(G) + \frac{1}{2}\, n\ r\ \omega^{*}(G) \quad .$$

AN APPLICATION

There have been several investigations about the possibility to reconstruct the matching polynomial of a graph G from either the Ulam subgraphs G-v (which is known to be possible [24]) or from the matching polynomials of the Ulam subgraphs (which still is an unsolved problem [25,26]). Theorems 2 and 4 make possible to formulate two related results.

Corollary 2.3. The matching polynomial of a graph G can be reconstructed from the matching polynomials of the subgraphs G-u-v, where u and v are adjacent vertices. Therefore the matching polynomial can be reconstructed also from the subgraphs G-u-v.

Proof. Using the fact that for all graphs G, $\alpha^{*}(G,\ 0) = 1$, we deduce from eq. (4)

$$\alpha^{*}(G,x) = 1 + \sum_{e(u,v)} \int_{0}^{x} \alpha^{*}(G-u-v,x)\ dx \quad .$$

If $\alpha^{*}(G)$ is known then $\alpha(G)$ can easily be obtained (and vice versa). Therefore in Corollary 2.3 the actual form of the matching polynomial needs not be specified. ■

Corollary 4.5. The independence polynomial of a graph G can be reconstructed from the independence polynomials of the subgraphs $G-N_v$. Therefore the independence polynomial can be reconstructed also from the subgraphs $G-N$.

Proof is same as in the previous case, except that it usues the identity

$$\omega^{*}(G,x) = 1 + \sum_{v} \int_{0}^{x} \omega^{*}(G-N_{v},x)\, dx \quad . \quad ■$$

Corollaries 2.3 and 4.5 reveal a somewhat paradoxical situation: Whereas the reconstruction of both the independence and the matching polynomials from Ulam subgraphs is difficult (and not yet solved), the reconstruction from smaller (and thus simpler) subgraphs is quite easy.

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REFERENCES

[1] A.Motoyama and H.Hosoya, J.Math.Phys. **18**, 1485 (1977).

[2] K.Balasubramanian and R.Ramaraj, J.Comput.Chem. **6**, 446 (1985).

[3] I.Gutman, Z.Naturforsch. **37a**, 69 (1982).

[4] W.C.Herndon and H.Hosoya, Tetrahedron **40**, 3987 (1984).

[5] I.Gutman and F.Harary, Utilitas Math. **24**, 97 (1983).

[6] C.Hoede and X.L.Li, Memor.Fac.Appl.Math.Univ.Twente **982**, 1 (1991).

[7] I.Gutman and S.J.Cyvin, Introduction to the Theory of Benzenoid Hydrocarbons, Springer-Verlag, Berlin 1989, pp. 108-111.

[8] C.Domb and M.S.Green (Eds.), Phase Transitions and Critical Phenomena, Academic Press, London 1972 and the subsequent volumes of this series.

[9] D.A.Lichtman and R.B.McQuistan, J.Math.Phys. **8**, 2441 (1967); R.B. McQuistan, J.Math.Phys. **14**, 1258 (1973).

[10] D.Cvetković, M.Doob, I.Gutman and A.Torgašev, Recent Results in the Theory of Graph Spectra, North-Holland, Amsterdam 1988, chapter 4.

[11] H.Hosoya, Bull.Chem.Soc.Japan **44**, 2332 (1971).

[12] O.J.Heilmann and E.H.Lieb, Commun.Math.Phys. **25**, 190 (1972).

[13] I.Gutman, M.Milun and N.Trinajstić, Match **1**, 171 (1975); J.Amer. Chem.Soc. **99**, 1692 (1977); I.Gutman, Publ.Inst.Math. (Beograd) **22**, 63 (1977).

[14] J.Aihara, J.Amer.Chem.Soc. **98**, 2750 (1976)

[15] E.J.Farrell, J.Comb.Theory **27B**, 75 (1979); Ars Combinatoria **9**, 221 (1980).

[16] I.Gutman, Match **6**, 75 (1979).

[17] D.Bonchev and D.H.Rouvray (Eds.), Chemical Graph Theory - Introduction and Fundamentals, Gordon & Breach, New York 1991, chapter 4.

[18] H.Hosoya, Discrete Appl.Math. **19**, 239 (1988).

[19] I.Gutman and H.Hosoya, Theor.Chim.Acta **48**, 279 (1978).

[20] P.Krivka, R.B.Mallion and N.Trinajstić, J.Mol.Struct. (Theochem) **164**, 363 (1988).

[21] F.H.Clarke, Discrete Math. **3**, 305 (1972).

[22] I.Gutman and O.E.Polansky, Theor.Chim.Acta **60**, 203 (1981).

[23] I.Gutman, Bull.Acad.Serbe Sci.Arts, in press.

[24] W.T.Tutte, in: J.A.Bondy and U.S.R.Murty (Eds.), Graph Theory and Related Topics, Academic Press, New York 1979, pp. 15-33.

[25] E.J.Farrell and J.C.Grell, Caribb.J.Math. **1**, 109 (1983); E.J.Farrell and C.M. de Matas, Internat.J.Math.Sci. **2**, 87 (1988).

[26] S.A.Wahid, Ph.D.Thesis, Univ.West Indies, St.Augustine, 1990.