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SOME RELATIONS FOR THE μ-POLYNOMIAL

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Abstract: If G and H are two graphs, g_1 and g_2 vertices of G, h_1 and h_2 vertices of H, then G:H is obtained by identifying g_i with h_i, i=1,2. Recurrence relations for the μ-polynomial of G:H are deduced and some applications to the theory of S- and T-topomers given. An unsolved problem concerning μ-polynomials is pointed out.

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Introduction

The μ-polynomial concept was introduced and elaborated in [1]. It provides a unification of two important graph-theoretical polynomials, namely of the characteristic and the matching polynomial.

Let G be a graph. Then its μ-polynomial $\mu(G)$ is defined as [1]:

$$\mu(G) = \sum_{s} (-1)^{c(s)} \, 2^{r(s)} \, x^{n-n(s)} \, T(s) \tag{1}$$

where s is a Sachs graph and the summation goes over the set $\underline{\underline{S}}(G)$ of all the Sachs graphs which are as subgraphs contained in the graph G. For other symbols used in (1) the reader should consult ref. [1].

In the following we shall write eq. (1) in an abbreviated form as

$$\mu(G) = \mathrm{sum}[\underline{\underline{S}}(G)] \quad . \tag{2}$$

If G contains the cycles $Z_1, Z_2, \ldots, Z_r$ then $\mu(G)$ depends on a vector $\underline{\underline{t}} = (t_1, t_2, \ldots, t_r)$ whose component t_a is a variable weight associated with the cycle Z_a , $a=1,2,\ldots,r$. For $\underline{\underline{t}} = \underline{\underline{1}}$ (i.e. for $t_1 = t_2 = \cdots = t_r = 1$) the μ-polynomial reduces to the characteristic polynomial. For $\underline{\underline{t}} = \underline{\underline{0}}$ (i.e. for $t_1 = t_2 = \cdots = t_r = 0$) the μ-polynomial gives as another special case the matching polynomial. If the graph G is acyclic $(r = 0)$, then the μ-, the matching and the characteristic polynomials of G coincide.

The fundamental properties of the μ-polynomial are exposed in [1]. Further results along the same lines can be found in [2-7]. Because of its dependence on the vector $\underline{\underline{t}}$, the μ-polynomial is especially suitable for modeling the effect of cyclic conjugation on various π-electron quantities [1,8-11].

In the present paper we offer some further relations for the μ-polynomial and point out an application of the results obtained to the theory of S- and T-topomers.

Preliminaries

In [1] the following recurrence relation for the μ-polynomial (called Corollary 4.3) was given without proof. Let g_1 and h_1 be two vertices of the graphs G and H, respectively and let G·H be obtained by identifying g_1 with h_1. Then

$$\mu(G\cdot H) = \mu(G)\ \mu(H_1) + \mu(G_1)\ \mu(H) - x\ \mu(G_1)\ \mu(H_1) \qquad (3)$$

where $G_1 = G-g_1$, $H = H-h_1$.

The proof of (3) is simple. Denote the vertex obtained by identifying g_1 with h_1 by f_1. Now the set $\underline{\underline{S}}(G\cdot H)$ can be partitioned into disjoint subsets $\underline{\underline{S}}_g(G\cdot H)$, $\underline{\underline{S}}_h(G\cdot H)$ and $\underline{\underline{S}}_o(G\cdot H)$, such that

$\underline{\underline{S}}_g(G\cdot H)$ = set of the Sachs graphs of G·H in which the vertex f_1 belongs to a component which is entirely in G;

$\underline{\underline{S}}_h(G\cdot H)$ = set of the Sachs graphs of G·H in which the vertex f_1 belongs to a component which is entirely in H;

$\underline{\underline{S}}_o(G\cdot H)$ = set of the Sachs graphs of G·H which do not contain the vertex f_1.

From these definitions is immediate that

$$\underline{\underline{S}}_g(G\cdot H) \cup \underline{\underline{S}}_o(G\cdot H) = \underline{\underline{S}}(G \dot{+} H_1)$$

$$\underline{\underline{S}}_h(G\cdot H) \cup \underline{\underline{S}}_o(G\cdot H) = \underline{\underline{S}}(G_1 \dot{+} H)$$

$$\underline{\underline{S}}_o(G\cdot H) = \underline{\underline{S}}(K_1 \dot{+} G_1 \dot{+} H_1)$$

where K_1 is the one-vertex graph. (In the above formula, the unique vertex of K_1 corresponds to the vertex f_1.) Here and later $G_a \dot{+} G_b$ denotes the graph whose components are G_a and G_b. Using (2) we now have

$$\mu(G\cdot H) = \mathrm{sum}[\underline{\underline{S}}_g(G\cdot H) \cup \underline{\underline{S}}_h(G\cdot H) \cup \underline{\underline{S}}_o(G\cdot H)] =$$

$$= \mathrm{sum}[\underline{\underline{S}}_g(G\cdot H) \cup \underline{\underline{S}}_o(G\cdot H)] + \mathrm{sum}[\underline{\underline{S}}_h(G\cdot H) \cup \underline{\underline{S}}_o(G\cdot H)] -$$

$$- \mathrm{sum}[\underline{\underline{S}}_o(G\cdot H)] \quad .$$

Hence

$$\mu(G\cdot H) = \mu(G \dot{+} H_1) + \mu(G_1 \dot{+} H) - \mu(K_1 \dot{+} G_1 \dot{+} H_1) \qquad (4)$$

from which formula (3) follows when one uses the facts that [1]

$$\mu(G_a \dot{+} G_b) = \mu(G_a)\ \mu(G_b) \qquad (5)$$

and $\mu(K_1) = x$.

The crucial step in the above proof is the partitioning of $\underline{\underline{S}}(G\cdot H)$ into $\underline{\underline{S}}_g(G\cdot H)$, $\underline{\underline{S}}_h(G\cdot H)$ and $\underline{\underline{S}}_o(G\cdot H)$. This is possible because the vertex f_1 is a cutpoint and therefore there are no Sachs graphs of $G\cdot H$ in which f_1 belongs to a component (= a cycle) which is partially in G and partially in H.

The μ-polynomial of the graph G:H

Formula (3) is concerned with a graph obtained by coalescing one pair of vertices. We shall now extend the consideration to the case where two pairs of vertices are simultaneously identified.

Let G be a graph and g_1 and g_2 its two distinct vertices. Let H be another graph and h_1 and h_2 its two distinct vertices. Construct the graph G:H by identifying g_i with h_i , i=1,2. The two newly formed vertices will be denoted by f_1 and f_2, respectively.

Our aim is to derive a recurrence relation for μ(G:H) as similar to (3) as possible. In order to achieve this goal, partition the set $\underline{\underline{S}}(G:H)$ with respect to the vertex f_1 in the same manner as before. In addition to $\underline{\underline{S}}_g(G:H)$, $\underline{\underline{S}}_h(G:H)$ and $\underline{\underline{S}}_o(G:H)$ we must now introduce a fourth subset, namely

$\underline{\underline{S}}_{gh}(G:H)$ = set of the Sachs graphs of G:H in which the vertex f_1 belongs to a component which is partially in G and partially in H.

Then

$$\underline{\underline{S}}(G:H) = \underline{\underline{S}}_g(G:H) \cup \underline{\underline{S}}_h(G:H) \cup \underline{\underline{S}}_o(G:H) \cup \underline{\underline{S}}_{gh}(G:H)$$

and furthermore

$$\underline{\underline{S}}_g(G:H) \cup \underline{\underline{S}}_o(G:H) = \underline{\underline{S}}(G \cdot H_1)$$

$$\underline{\underline{S}}_h(G:H) \cup \underline{\underline{S}}_o(G:H) = \underline{\underline{S}}(G_1 \cdot H)$$

$$\underline{\underline{S}}_o(G:H) = \underline{\underline{S}}(K_1 \dot{+} G_1 \cdot H_1)$$

where $G \cdot H_1$ denotes the graph obtained by identifying the vertex g_2 of G with the vertex h_2 of H_1 ; the graphs $G_1 \cdot H$ and $G_1 \cdot H_1$ are defined analogously.

The situation with the set $\underline{\underline{S}}_{gh}(G:H)$ is slightly more complicated. If $s \in \underline{\underline{S}}_{gh}(G:H)$, then the component of s to which f_1 belongs is necessarily a cycle. Bearing in mind the way in which G:H has been constructed, we conclude that every such cycle must pass through both f_1 and f_2. Therefore an arbitrary such cycle, say Z_{ab} , can be viewed as obtained by combining a certain path P_a , which connects the vertices g_1 and g_2 of G with another path P_b , which connects the vertices h_1 and h_2 of H. Furthermore, $G:H-Z_{ab} = (G-P_a) \dot{+} (G-P_b)$.

Applying (1) we conclude that

$$\mathrm{sum}[\underline{\underline{S}}_{gh}(G:H)] = -2 \sum_{ab} t_{ab} \, \mathrm{sum}[\underline{\underline{S}}(G:H-Z_{ab})] =$$

$$= -2 \sum_a \sum_b t_{ab} \, \mu(G-P_a) \, \mu(H-P_b)$$

where t_{ab} is the weight associated with the cycle Z_{ab}. The double summation in the latter equation embraces all pairs of the previously specified paths P_a, P_b.

Substituting the above relations into the identity

$$\mu(G:H) = \mathrm{sum}[\underline{\underline{S}}_g(G:H) \cup \underline{\underline{S}}_o(G:H)] + \mathrm{sum}[\underline{\underline{S}}_h(G:H) \cup \underline{\underline{S}}_o(G:H)] -$$

$$- \mathrm{sum}[\underline{\underline{S}}_o(G:H)] + \mathrm{sum}[\underline{\underline{S}}_{gh}(G:H)]$$

we reach one of our main results:

$$\mu(G{:}H) = \mu(G\cdot H_1) + \mu(G_1\cdot H) - \mu(K_1 \dotplus G_1\cdot H_1) - \\ - 2 \sum_a \sum_b t_{ab}\, \mu(G-P_a)\, \mu(H-P_b) \tag{6}$$

which should be compared with eq.(4). Of course, $\mu(K_1 \dotplus G_1\cdot H_1) = x\, \mu(G_1\cdot H_1)$.

As a matter of fact, eq. (3) is a special case of (6). Namely, when g_2 and h_2 are not identified, then $G\cdot H_1 = G \dotplus H_1$, $G_1\cdot H = G_1 \dotplus H$ and $G_1\cdot H_1 = G_1 \dotplus H_1$, and the relation (5) can be used. Since there are no cycles of the type Z_{ab} , the double sum in (6) vanishes. Then (3) follows from (6).

The recursion relation (3) can be applied to the first three polynomials on the right-hand side of (6) and an elementary calculation gives our final result:

$$\mu(G{:}H) = \mu(G)\mu(H_{12}) + \mu(G_1)\mu(H_2) + \mu(G_2)\mu(H_1) + \mu(G_{12})\mu(H) - \\ - x[\mu(G_1)\mu(H_{12}) + \mu(G_2)\mu(H_{12}) + \mu(G_{12})\mu(H_1) + \mu(G_{12})\mu(H_2)] + \\ + x^2\, \mu(G_{12})\mu(H_{12}) - 2 \sum_a \sum_b t_{ab}\, \mu(G-P_a)\mu(H-P_b) \quad , \tag{7}$$

where $G_{12} = G-g_1-g_2$ and $H_{12} = H-h_1-h_2$.

Application: Topomers

Let A be a graph and p and q its two non-equivalent vertices. Let B be another graph and r and s its two non-equivalent vertices. Construct the graph S* by identifying p with r and q with s. Construct the graph T* by identifying p with s and q with r. Then

$$\mu(T^*) - \mu(S^*) = \{\mu(A-p) - \mu(A-q)\}\{\mu(B-r) - \mu(B-s)\} . \quad (8)$$

Since the graphs S^* and T^* are both of the type G:H, one may apply eq. (7) to them. Formula (8) follows then straightforwardly.

Let S (respectively T) be obtained from A and B by joining the vertices p with r and q with s (respectively p with s and q with r). As a consequence of (8) we have then

$$\mu(T) - \mu(S) = \{\mu(A-p) - \mu(A-q)\}\{\mu(B-r) - \mu(B-s)\} . \quad (9)$$

Note that the right-hand sides of (8) and (9) are identical.

In order to see that (9) is a special case of (8) consider the auxiliary graph A^{pq}, obtained from A by attaching a new vertex to each p and q. Let these new vertices be labeled by p' and q', respectively. One should now observe that S (respectively T) can be constructed from A^{pq} and B by identifying the vertex p' with r and q' with s (respectively p' with s and q' with r). This enables the application of (8), viz.,

$$\mu(T) - \mu(S) = \{\mu(A^{pq}-p') - \mu(A^{pq}-q')\}\{\mu(B-r) - \mu(B-s)\} .$$

Eq. (9) is now a consequence of the relations

$$\mu(A^{pq}-p') = x\,\mu(A) - \mu(A-q)$$

and

$$\mu(A^{pq}-q') = x\,\mu(A) - \mu(A-p) \quad .$$

Formula (9) was first derived in [2]. The special cases of formula (8) for $\underline{\underline{t}} = \underline{\underline{1}}$ (characteristic polynomial) and for $\underline{\underline{t}} = \underline{\underline{0}}$

(matching polynomial) were recently obtained using a different way of reasoning [12].

We wish to point here at a generalization of (8). Suppose that the edges of A and B are weighted so that all edges incident to p,q,r and s have weight k_p, k_q, k_r and k_s, respectively. These weighted graphs will be denoted by A_k and B_k, respectively and the corresponding topomer graphs by S_k^* and T_k^*. Of course, for $k_p = k_q = k_r = k_s = 1$ the weighted graphs A_k, B_k, S_k^* and T_k^* coincide with the simple graphs A, B, S^* and T^*, respectively.

It can be proved that instead of (8) we have

$$\mu(T_k^*) - \mu(S_k^*) = \{k_q^2[\mu(A-p) - x\,\mu(A-p-q)] -$$

$$- k_p^2[\mu(A-q) - x\,\mu(A-p-q)]\}\{k_s^2[\mu(B-r) - x\,\mu(B-r-s)] -$$

$$- k_r^2[\mu(B-s) - x\,\mu(B-r-s)]\}$$

whose special case for $k_p = k_q = k_r = k_s = k$ is

$$\mu(T_k^*) - \mu(S_k^*) = k^4[\mu(T^*) - \mu(S^*)] \ . \qquad (10)$$

For the topomer graphs S and T a reasonable weighting is to associate weight k_p and k_q to the edges of A^{pq}, connecting p with p′ and q with q′, respectively, and to assume that all other edges have normal (= unit) weight. Then a reasoning analogous to that used to deduce eq. (9) yields

$$\mu(T_k) - \mu(S_k) = \{k_p^2\,\mu(A-p) - k_q^2\,\mu(A-q)\}\{\mu(B-r) - \mu(B-s)\}$$

which for $k_p = k_q = k$ becomes

$$\mu(T_k) - \mu(S_k) = k^2[\mu(T) - \mu(S)] \quad . \tag{11}$$

The special cases of formulas (10) and (11) for $\underline{\underline{t}} = \underline{\underline{1}}$ and $\underline{\underline{t}} = \underline{\underline{0}}$ played an important role in the proof of the TEMO interlacing relations [12,13].

A problem

If G is a graph and g_1 and g_2 are two of its vertices, then the equality (12) is known for the characteristic polynomial ϕ [14, 15,16] and a similar relation (13) for the matching polynomial α [17]:

$$\phi(G_1)\phi(G_2) - \phi(G)\phi(G_{12}) = [\sum_a \phi(G-P_a)]^2 \tag{12}$$

$$\alpha(G_1)\alpha(G_2) - \alpha(G)\alpha(G_{12}) = \sum_a [\alpha(G-P_a)]^2 \quad . \tag{13}$$

The notation in (12) and (13) is same as in the previous sections: $G_1 = G-g_1$, $G_2 = G-g_2$, $G_{12} = G-g_1-g_2$; P_a is a path connecting g_1 and g_2 and the summations range over all such paths.

What would be the μ-polynomial equivalent of the formulas (12) and (13) ? This seems to be a difficult problem.

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