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ON A RECURSIVE POLYNOMIAL GRAPH INVARIANT FOR CHAINS OF POLYGONS*)

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Introduction

Polynomial graph invariants have found interesting applications in organic chemistry and biology for characterization molecular graphs and DNA [1-5]. These applications stimulates intensive theoretical studies of polynomial invariants.In this paper we consider a general calculation scheme of one type polynomial invariant for classes of polygon graphs. A graph of such class may be presented as n-gons in a plane connected with each other by an edge. Some of these classes include molecular graphs of polycyclic chemical compounds. The scheme is based on recurrent relations which are induced by two elementary graph operations: deletion and contraction of an edge. By a simple way we present a general explicit formulae for the polynomial. Then we show that several well known polynomials may by injected into this scheme with suitable coefficients.By construction the polynomials are similar to the dichromate of Tutte, i.e. they don't distinguish 2-isomorphic graphs. There-

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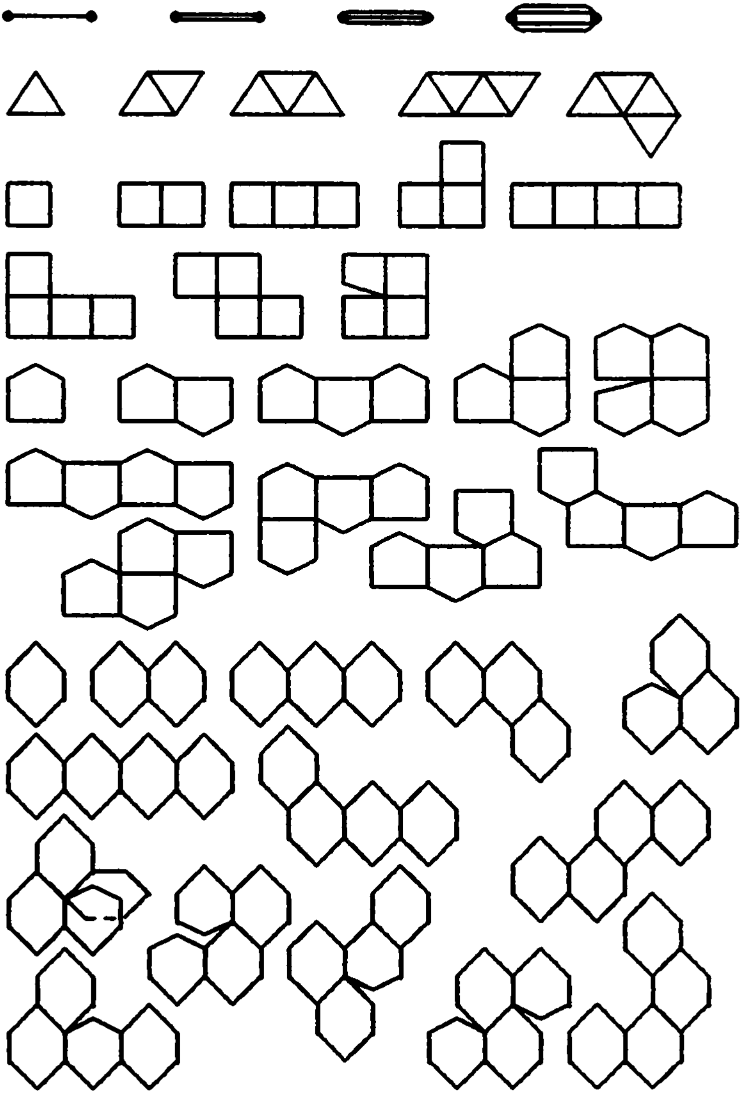

Fig. 1. All graphs of U_k^n, where $n \leq 6$ and $k \leq 4$.

fore they characterize a whole class of considered graphs with equal numbers of n-gons.

1. Basic notations and definitions

All graphs considered in this paper are finite, undirected, connected, with or without loops or multiple edges. If G is a graph, V(G) and E(G) will denote its sets of vertices and edges, $|V(G)| = p$ and $|E(G)| = q$. The graphs called chains of n-gons consist of n-gons connected with each other by edges. Two arbitrary n-gons either have only a common edge (i.e. they are adjacent), or have no common vertices. Each n-gon is adjacent to no more than two other n-gons and no three n-gons which share a common edge. Two terminal n-gons of a chain are adjacent to exactly one other n-gon. Let U_k^n be the class of all chains with k copies of n-gons. Then graphs of U_k^n may be defined by recursion. We assume that U_o^n, $n \geq 2$, consists of the degenerate n-gon which is the tree with a single edge on two vertices. Every $G \in U_k^n$, $k \geq 1$, $n \geq 2$, is obtained from some $H \in U_{k-1}^n$ by identifying an edge of a new n-gon with an edge of the terminal n-gons in H. A chain of U_k^n may be embedded into the plane such that all its interior faces will be n-gons. All graphs of U_k^n for $2 \leq n \leq 6$ and $1 \leq k \leq 4$ are presented on Fig. 1.

We remark that the class U_k^n contains graphs which play an important role in organic chemistry. Let C_k^n be subset of graphs of U_k^n, for which each vertex is common not more than for two n-gons. Therefore the degree of any vertex of graph of C_k^n equals two or three. Graphs of C_k^6 are well-known as molecular graphs of unbranched catacondensed aromatic hydrocarbons [1,2,6]. Moreover there is one-to-one correspondence between graphs of classes U_k^n and C_k^{n+2}. In particular, for classes U_k^3 and U_k^4 we have [7,8]:

$$|U_k^3| = \begin{cases} 2^{k-4} + 2^{(k-4)/2}, & \text{if } k \geq 4 \text{ even}, \\ 2^{k-4} + 2^{(k-5)/2}, & \text{if } k \geq 5 \text{ odd} \end{cases}$$

and

$$|U_k^4| = \begin{cases} (3^{(k-2)/2} + 1)^2/4, & \text{if } k \geq 2 \text{ even}, \\ (3^{k-2} + 3^{(k-1)/2} + 3^{(k-3)/2} + 1)/4, & \text{if } k \geq 3 \text{ odd}. \end{cases}$$

In general case the numbers of all graphs in U_k^n are given by the following compact expression ($k > 1$, $n > 5$) [9]:

$$|U_k^{n-2}| = \frac{1}{4}(n-3)^{k-2} + \frac{1}{8}[1+(-1)^n] + \frac{1}{8}[1-(-1)^n]C_2^k +$$
$$+ \frac{1}{4}\{1+(-1)^n + \frac{1}{2}[1-(-1)^n][1+(-1)^k] +$$
$$+ [1-(-1)^k]\lfloor (n-3)/2 \rfloor\}(n-3)^{\lfloor k/2 \rfloor - 1}.$$

Two graphs are said to be 2-isomorphic if there is a bijection between its edges which induces a one-to-one correspondence between its cycles [10]. It easy to see that two arbitrary chains of U_k^n are 2-isomorphic graphs.

We recall two well-known polynomial invariants for graphs. The dichromate of Tutte $\chi(G;x,y)$ of a graph G is defined by the following equality [11]:

$$\chi(G;x,y) = (x-1)^{-\omega(G)} \sum_{Y \subset E(G)} (x-1)^{\omega(G-Y)}(y-1)^{\beta(G-Y)},$$

where the summation goes over all edge subsets Y of $E(G)$, $\omega(G)$ is the number of connected components in G, and $\beta(G)$ is the cyclomatic number of a graph: $\beta(G) = q(G) - p(G) + \omega(G)$.

The polynomial $N(G;t,x,y)$ of a graph G was introduced by Negami in [12]: $N(G;t,x,y) = \sum_{Y \subset E(G)} t^{\omega(G-Y)} x^{q(G-Y)} y^{q(Y)}$.

We will present recurrent relations and explicit formulae for the dichromate of Tutte and Negami's polynomial for graphs of U_k^n.

2. The 2-invariant function

We now define a function f by a recursive scheme with formal coefficients. Our aim is to derive an explicit formula of f for chains of n-gons. As elementary operation of connected graphs, we consider the deletion and the contraction of edges. We denote the resulting graph of deletion and contraction of an edge e by G-e and G/e respectively. A graph G/e is obtained from G by deleting e and identifying its ends to a single vertex. An edge is called the isthmus if its removal increases the number of connected components in a graph. A graph function is called a 2-invariant if it assigns to 2-isomorphic graphs the same value.

Let f be a 2-invariant graph function with values from some ring R. We will assume that a function f satisfies the following conditions:

1) if an edge e is not a loop or an isthmus, then

$$f(G) = Af(G/e) + Bf(G-e), \tag{1}$$

where the coefficients A and B don't depend on the choice of e;

2) if H·K is a union of two subgraphs H and K which have only a common vertex, then

$$f(H\cdot K) = Cf(H)f(K), \tag{2}$$

where the coefficint C does not depend on the subgraphs H and K;

3) if a graph T_1 is a tree with a single edge on two vertices, then

$$f(T_1) = D; \tag{3}$$

4) if a graph L_1 is a single vertex with only loop, then

$$f(L_1) = E. \tag{4}$$

Applying the above properties of the function f, we may immediately calculate f for the simplest classes of graphs.

If a graph T_q is a connected tree with q edges, then

$$f(T_q) = C^{q-1}D^q. \tag{5}$$

If a graph L_q is a single vertex with q edges, then

$$f(L_q) = C^{q-1}E^q.$$

If a graph D_q consists of two vertices joining by multiple q edges, then

$$f(D_q) = B^{q-1}D + AE\,\frac{B^{q-1} - (CE)^{q-1}}{B - CE}.$$

If a graph C_q is a simple cycle with q edges, then

$$f(C_q) = A^{q-1}E + BD\,\frac{A^{q-1} - (CD)^{q-1}}{A - CD}. \tag{6}$$

3. Function f for graphs of U_k^n

Since the function f is 2-invariant, we shall denote the value f(G) for an arbitrary graph $G \in U_k^n$ by f_k^n. Recall that the class U_o^n, $n \geqq 2$, contains the degenerate n-gons. Then by (3)

$$f_o^n = f(T_1) = D. \tag{7}$$

Furthermore, the class U_1^n, $n \geqq 2$, contains an n-gon only. By (6)

$$f_1^n = f(C_n) = A^{n-1}E + BD\,\frac{A^{n-1} - (CD)^{n-1}}{A - CD}. \tag{8}$$

The following theorem gives a recurrent formula of the function f for chains of n-gons.

THEOREM 1. For a chain with k n-gons, $n \geq 2$ and $k \geq 2$, we have:

$$f_k^n = \left\{ B \frac{A^{n-1} - (CD)^{n-1}}{A - CD} + A^{n-2}CE \right\} f_{k-1}^n - $$
$$- A^{n-2}BC^{n-1}D^{n-2}Ef_{k-2}^n. \qquad (9)$$

PROOF. Let $G_k^n \in U_k^n$. Consider a calcualation scheme for $f(G_k^n)$ presented on Fig.2. Graph H_k^n is obtain from G_k^n by contracting an edge of its terminal n-gon. Graph $G_{k-1}^n \cdot T_{n-2}$ is constructed from G_k^n by deleting the edge. Using (1),(2) and (5), we have

$$f_k^n = Af(H_k^n) + Bf(G_{k-1}^n \cdot T_{n-2}) =$$
$$= Af(H_k^n) + B(CD)^{n-2}f(G_{k-1}^n).$$

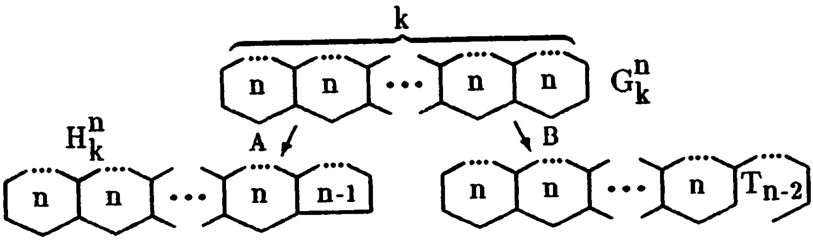

Fig.2. Calculation scheme for G_k^n .

Hence

$$f(H_k^n) = \frac{1}{A} (f_k^n - B(CD)^{n-2}f_{k-1}^n). \qquad (10)$$

Consider now a calculation scheme for $f(H_k^n)$ shown on Fig.3. In this case we can written $f(H_k^n)$ through the function f for graphs $H_{k-1}^n \cdot L_1$, G_{k-1}^n and $G_{k-1}^n \cdot T_i$ for $1 \leq i \leq n-3$.

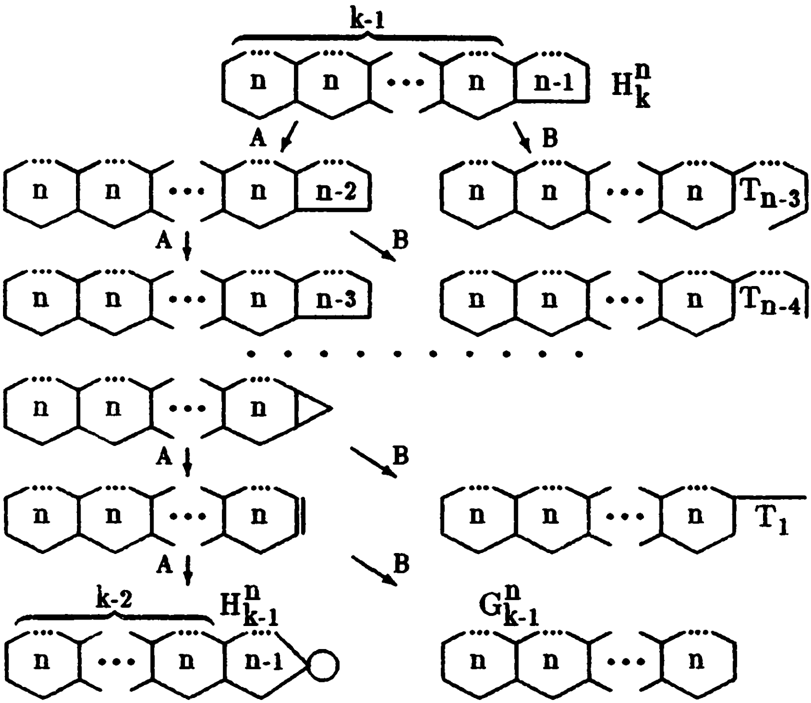

Fig.3. Calculation scheme for H^n_k.

From (1), (2) and (5), we have

$$
\begin{aligned}
f(H^n_k) &= A^{n-2} f(H^n_{k-1}\cdot L_1) + B \sum_{i=0}^{n-4} A^i f(G^n_{k-1}\cdot T_{n-3-i}) + \\
&+ BA^{n-3} f(G^n_{k-1}) = A^{n-2} CEf(H^n_{k-1}) + \\
&+ B \left[\sum_{i=0}^{n-3} A^i (CD)^{n-3-i} \right] f(G^n_{k-1}) = \\
&= A^{n-2} CEf(H^n_{k-1}) + B \frac{A^{n-2} - (CD)^{n-2}}{A - CD} f^n_{k-1} \,. \qquad (11)
\end{aligned}
$$

Substituting $f(H_k^n)$ and $f(H_{k-1}^n)$ from (10) into (11) and writing f_k^n through f_{k-1}^n and f_{k-2}^n, we obtain

$$f_k^n = \left\{ B(CD)^{n-2} + A^{n-2}CE + AB\,\frac{A^{n-2} - (CD)^{n-2}}{A - CD} \right\} f_{k-1}^n -$$
$$- A^{n-2}CEB(CD)^{n-2} f_{k-2}^n =$$
$$= \left\{ B\,\frac{A^{n-1} - (CD)^{n-1}}{A - CD} + A^{n-2}CE \right\} f_{k-1}^n -$$
$$- A^{n-2}BC^{n-1}D^{n-2}Ef_{k-2}^n .$$

This completes the proof. □

Note that the expressions at f_{k-1}^n and f_{k-2}^n in (9) don't depend on k. Denote these coefficients by a_n and b_n:

$$a_n = B\,\frac{A^{n-1} - (CD)^{n-1}}{A - CD} + A^{n-2}CE,$$

$$b_n = A^{n-2}BC^{n-1}D^{n-2}E.$$

Hence the formula (9) may be written in the form

$$f_k^n = a_n f_{k-1}^n - b_n f_{k-2}^n .$$

Substituting the analogous expression for f_{k-1}^n and f_{k-2}^n into the later equation, we have

$$f_k^n = a_n(a_n f_{k-2}^n - b_n f_{k-3}^n) - b_n f_{k-2}^n =$$
$$= (a_n^2 - b_n) f_{k-2}^n - a_n b_n f_{k-3}^n.$$

Repeating this process, we can present f_k^n through f_i^n and f_{i-1}^n for an arbitrary $1 \le i \le k-1$. Denote by c_n^{k-i} and d_n^{k-i} the corresponding coefficients at f_i^n and f_{i-1}^n, where $c_n^1 = a_n$ and $d_n^1 = b_n$. This implies the following simple

LEMMA. For arbitrary $n \geqq 2$ and $1 \leq i \leq k-2$,

$$\begin{pmatrix} c_n^{i+1} \\ d_n^{i+1} \end{pmatrix} = \begin{pmatrix} a_n & -1 \\ b_n & 0 \end{pmatrix} \begin{pmatrix} c_n^{i} \\ d_n^{i} \end{pmatrix}.$$

Using (7) and (8), we get for the function f the following

THEOREM 2. For a chain with k n-gons, $n \geqq 2$ and $k \geqq 2$, we have:

$$f_k^n = c_n^{k-1} f_1^n - d_n^{k-1} f_o^n ,$$

where

$$f_o^n = D, \quad f_1^n = A^{n-1}E + BD \frac{A^{n-1} - (CD)^{n-1}}{A - CD} ,$$

$$\begin{pmatrix} c_n^{k} \\ d_n^{k} \end{pmatrix} = \begin{pmatrix} a_n & -1 \\ b_n & 0 \end{pmatrix}^{k-1} \begin{pmatrix} a_n \\ b_n \end{pmatrix},$$

$$a_n = A^{n-2}CE + B \frac{A^{n-1} - (CD)^{n-1}}{A - CD} , \quad b_n = A^{n-2}BC^{n-1}D^{n-2}E .$$

4. The dichromate of Tutte, Negami's and Yamada's polynomils

In this section we show that the properties of the func - tion f coincides with the properties of the dichromate of Tutte, Negami's and Yamada's polynomials for chains of n-gons. We also consider the chromatic and the flow polynomials. This allow to obtain recurrent relations and explicit formulae for the polynomials as a corollary of Theorems 1 and 2.

The dichromate of Tutte. It is well known that the dich - romate of Tutte $\chi(G;x,y)$ satisfies the following recursive relation for an arbitrary graph G [11]:

$$\chi(G;x,y) = \chi(G/e;x,y) + \chi(G-e;x,y),$$

where e is not a loop or an isthmus. Further, if subgraphs H and K have only a common vertex, then $\chi(H\cdot K;x,y) = \chi(H;x,y)\chi(K;x,y)$. For graphs T_1 and L_1 the dichromate is equal to $\chi(T_1;x,y) = x$ and $\chi(L_1;x,y) = y$. This polynomial is also a 2-invariant of graphs. Therefore, the properties of the dichromate are identical with the corresponding properties of the function f under the coefficients: A = 1, B = 1, C = 1, D = x, E = y. In this case for other quantities from Theorem 2, we have $a_n = y + \frac{1 - x^{n-1}}{1 - x}$, $b_n = yx^{n-2}$, $f_o^n = x$ and $f_1^n = y + x\frac{1 - x^{n-1}}{1 - x}$.

COROLLARY 1. For chains with k n-gons, the dichromate of Tutte satisfies the following recurrent relation

$$\chi(G_k^n;x,y) = \left(y + \frac{1-x^{n-1}}{1-x}\right)\chi(G_{k-1}^n;x,y) - yx^{n-2}\chi(G_{k-2}^n;x,y)$$

and it may be presented as

$$\chi(G_k^n;x,y) = c_n^{k-1}\left(y + x\frac{1-x^{n-1}}{1-x}\right) - d^{k-1}x,$$

where

$$\begin{pmatrix} c_n^k \\ d_n^k \end{pmatrix} = \begin{pmatrix} y + \frac{1-x^{n-1}}{1-x} & -1 \\ yx^{n-2} & 0 \end{pmatrix}^{k-1} \begin{pmatrix} y + \frac{1-x^{n-1}}{1-x} \\ yx^{n-2} \end{pmatrix}.$$

The polynomial of Negami. By construction, the polynomial of Negami N(G;t,x,y) is defined by the equation [12]:

$$N(G;t,x,y) = xN(G/e;t,x,y) + yN(G-e;t,x,y),$$

where e is an arbitrary edge of a graph G. For graphs $H\cdot K$,

T_1 and L_1, we have $N(H \cdot K;t,x,y) = \frac{1}{t} N(H;t,x,y)N(K;t,x,y)$, $N(T_1;t,x,y) = t(x+ty)$ and $N(L_1;t,x,y) = t(x+y)$. The polynomial is a 2-invariant of graphs. Hence, the properties of f and Negami's polynomial are the same under coefficients: $A = x$, $B = y$, $C = 1/t$, $D = t(x+ty)$, $E = t(x+y)$. For other quantities from Theorem 2, we have $a_n = \frac{1}{t}((x + ty)^{n-1} - x^{n-1}) + (x+y)x^{n-2}$, $b_n = x^{n-2}y(x+ty)^{n-2}(x+y)$, $f_o^n = t(x+ty)$ and $f_1^n = (x+ty)^n + (t-1)x^n$.

COROLLARY 2. For chains with k n-gons, the polynomial of Negami satisfies the following recurrent relation

$$N(G_k^n) = \left[(x+y)x^{n-2} + \frac{(x+ty)^{n-1} - x^{n-1}}{t} \right] N(G_{k-1}^n) - - y(x+y)x^{n-2}(x+ty)^{n-2}N(G_{k-2}^n)$$

and it may be presented in the form

$$N(G_k^n;t,x,y) = c_n^{k-1} f_1^n - d_n^{k-1} f_o^n,$$

where $f_o^n = t(x+ty)$, $f_1^n = (x+ty)^n + (t-1)x^n$,

$$\begin{bmatrix} c_n^k \\ d_n^k \end{bmatrix} = \begin{bmatrix} a_n & -1 \\ b_n & 0 \end{bmatrix}^{k-1} \begin{bmatrix} a_n \\ b_n \end{bmatrix},$$

$$a_n = \frac{1}{t}((x+ty)^{n-1} + (tx+ty-x)x^{n-2}),$$

$$b_n = y(x+y)x^{n-2}(x+ty)^{n-2}.$$

<u>The polynomial of Yamada.</u> This polynomial h(G)(x,y) satisfies the following recursive expression [13,14]:

$$h(G)(x,y) = h(G/e)(x,y) - \frac{1}{x} h(G-e)(x,y).$$

According to the properties of the polynomial, we have $h(G\cdot H)(x,y) = \frac{1}{x}h(G)(x,y)\cdot h(H)(x,y)$, $h(T_1)(x,y) = 0$ and $h(L_1)(x,y) = xy-1$.

Then we can conclude that the properties of f and $h(G)(x,y)$ coincide under the coefficients: $A=1$, $B=-1/x$, $C=1/x$, $D=0$, $E=xy-1$. For other quantities from Theorem 2, $a_n = y-2/x$, $b_n = 0$, $c_n^{k-1} = (a_n)^{k-1}$, $d_n^{k-1} = 0$, $f_o^n = 0$ and $f_1^n = xy-1$.

COROLLARY 3. For chains with k n-gons, the polynomial of Yamada satisfies the following recurrent relation

$$h(G_k^n)(x,y) = \left(y - \frac{2}{x}\right) h(G_{k-1}^n)(x,y)$$

and it may be presented in the form

$$h(G_k^n)(x,y) = \left(y - \frac{2}{x}\right)^k (xy - 1).$$

<u>The chromatic polynomial.</u> The chromatic polynomial $P(G;\lambda)$ is the well known polynomial invariant of graphs. A recursive formula under deleting and contracting an edge is as follow [11]:

$$P(G;\lambda) = -P(G/e;\lambda) + P(G-e;\lambda),$$

where e is not a loop. For graphs $H\cdot K$, T_1 and L_1, we have $P(H\cdot K;\lambda) = \frac{1}{\lambda} P(H;\lambda)P(K;\lambda)$, $P(T_1;\lambda) = \lambda(\lambda-1)$ and $P(L_1;\lambda) = 0$. Therefore, the properties of f and $P(G;\lambda)$ coincide under the coefficients: $A = -1$, $B = 1$, $C = 1/\lambda$, $D = \lambda(\lambda-1)$, $E = 0$. Besides, we can write $a_n = \frac{1}{\lambda}((\lambda-1)^{n-1} - (-1)^{n-1})$, $b_n = 0$, $c_n^{k-1} = a_n^{k-1}$, $d_n^{k-1} = 0$, $f_o^n = \lambda(\lambda-1)$ and $f_1^n = \lambda(\lambda-1)a_n$.

As a result we obtain the simple formulae which also follow from other properties of the polynomial [11]. Namely, the chromatic polynomial satisfies the following recursive relation for chains with k n-gons:

$$P(G_k^n;\lambda) = \frac{1}{\lambda}[(\lambda-1)^{n-1} - (-1)^{n-1}]P(G_{k-1}^n;\lambda)$$

and it may be presented in the form

$$P(G_k^n;\lambda) = \frac{1}{\lambda^{k-1}}(\lambda-1)[(\lambda-1)^{n-1} - (-1)^{n-1}]^k.$$

The flow polynomial. For the flow polynomial $F(G;\lambda)$, the recursive formulae is written as [11]

$$F(G;\lambda) = F(G/e;\lambda) - F(G-e;\lambda),$$

where e is not a loop. Further, for graphs $H\cdot K$, T_1 and L_1, the equations $F(H\cdot K;\lambda) = F(H;\lambda)F(K;\lambda)$, $F(T_1;\lambda) = 0$ and $F(L_1;\lambda) = \lambda-1$ hold. Then the properties of f and $F(G;\lambda)$ are the same under the coefficients: $A = 1$, $B = -1$, $C = 1$, $D = 0$, $E = \lambda - 1$. For other quantities from Theorem 2, $a_n = \lambda-2$, $b_n = 0$, $c_n^{k-1} = a_n^{k-1}$, $d_n^{k-1} = 0$, $f_o^n = 0$ and $f_1^n = \lambda-1$. Hence, the flow polynomial satisfies the following recurrent relation for chains with k n-gons: $F(G_k^n;\lambda) = (\lambda-2)F(G_{k-1}^n;\lambda)$. This immediately implies $F(G_k^n;\lambda) = (\lambda-2)^{k-1}(\lambda-1)$. Notice that the flow polynomial is the specific case of of Yamada's polynomial at $x = 1$ and $y = \lambda$.

Table

Polynomial	A	B	C	D	E
The dichromate of Tutte $\chi(G;x,y)$	1	1	1	x	y
The polynomial of Negami $N(G;t,x,y)$	x	y	$\frac{1}{t}$	$t(x+ty)$	$t(x+y)$
The polynomial of Yamada $h(G)(x,y)$	1	$-\frac{1}{x}$	$\frac{1}{x}$	0	$xy-1$
The chromatic polynomial $P(G;\lambda)$	-1	1	$\frac{1}{\lambda}$	$\lambda(\lambda-1)$	0
The flow polynomial $F(G;\lambda)$	1	-1	1	0	$\lambda-1$

Now we present values of coefficients for all considered polynomials (see table):

$$f(G) = Af(G/e) + Bf(G-e);$$
$$f(H\cdot K) = Cf(H)f(K);$$
$$f(T_1) = D;$$
$$f(L_1) = E.$$

Conclusion

We have considered a general calculation scheme for the polynomial graph invariant based on edge deletion and contraction in a graph. For chains of polygons recurrent and explicit formulae of the invariant was derived. It was shown that some well-know polynomials are injected into this scheme with suitable coefficients. As a consequence, the formulae for the dichromate of Tutte and Negami's polynomial was presented.

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