Journal of Mathematical Chemistry 9(1992)381–387

Note

ON THE Z-COUNTING POLYNOMIAL FOR EDGE-WEIGHTED GRAPHS*

Sonja NIKOLIĆ, Dejan PLAVŠIĆ and Nenad TRINAJSTIĆ
The Rugjer Bošković Institute, P.O. Box 1016, 71001 Zagreb, The Republic of Croatia

Received 20 November 1991; revised 6 January 1992

Abstract

The construction of the Z-counting polynomial for edge-weighted graphs is discussed.

The Z-counting polynomial $Q(G;x)$ of a graph G was introduced two decades ago by Hosoya [1]. It is defined as

$$Q(G;x) = \sum_{k=0}^{[N/2]} p(G;k)x^k, \tag{1}$$

where the coefficient $p(G;k)$ represents the number of ways in which k non-adjacent edges can be chosen from G. Note that $p(G;0) = 1$ by definition, $p(G;1) =$ the number of edges in G and $p(G;N/2) =$ the number of 1-factors in G.

The Z-counting polynomial has a number of interesting properties [2–4]. For example, the Z-counting polynomial is closely related to the acyclic (reference, matching) polynomial $P^{ac}(G;x)$ of G

$$P^{ac}(G;x) = \sum_{k=0,}^{[N/2]} (-1)^k p(G;k)x^{N-2k}, \tag{2}$$

which is the fundamental quantity in the topological resonance energy concept [2,5]. The acyclic polynomial has also found other uses [4,6–9]. The relationship between the Z-counting polynomial and the acyclic polynomial is given by

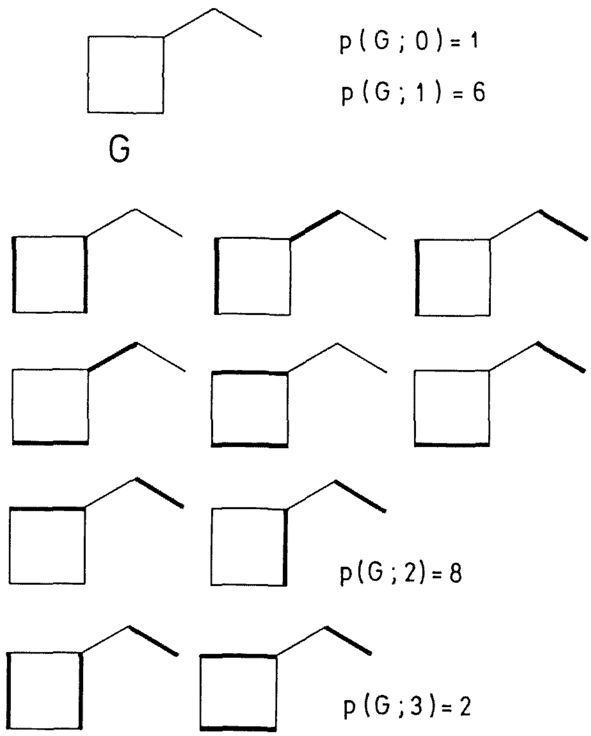
$$Q(G;x) = (-1)^k x^N P^{ac}(G; x = x^{-1}). \tag{3}$$

* Dedicated to Professor Haruo Hosoya (Tokyo) on the occasion of his 55th birthday for enriching chemical graph theory with the elegant concept of the Z-counting polynomial.

The major use of the Z-counting polynomial is for computing the Z-index $Z(G)$ of G[1] (hence the name):

$$Z(G) = \sum_{k=0}^{[N/2]} p(G;k) = Q(G; x = 1). \tag{4}$$

In fig. 1, we give as an example the "pedestrian" construction of the Z-counting polynomial for a graph G representing the carbon skeleton of vinylcyclobutadiene.



$Q(G;x) = 1 + 6x + 8x^2 + 2x^3$

Fig. 1. The construction of the Z-counting polynomial for a graph G depicting the carbon skeleton of vinylcyclobutadiene.

The corresponding acyclic polynomial is also immediately known:

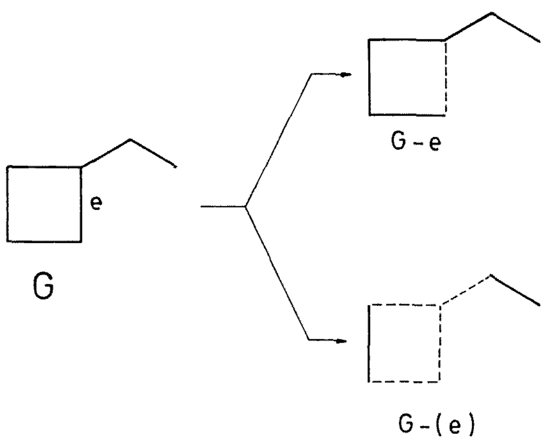
$$P^{ac}(G; x) = x^6 - 6x^4 + 9x^2 - 2. \tag{5}$$

The contributions to each $p(G; k)$ may be regarded as acyclic Sachs graphs [2,5,10] which are made up of only K_2 components [11].

The construction of the Z-counting polynomial via acyclic Sachs graphs is of great conceptual value, but computationally rather involved. For large graphs, the Z-counting polynomial cannot be constructed even by means of the computer. A much easier and faster way to compute the Z-counting polynomial is by the following recurrence relation:

$$Q(G; x) = Q(G - e; x) + xQ(G - (e); x), \tag{6}$$

which is the same type of expression as the one which is used for computing the acyclic polynomial. $G - e$ and $G - (e)$ in (6) represent subgraphs of G which are obtained by removing, respectively, an edge, and an edge and its incident vertices from G. The idea behind (6) is to reduce the graph G to smaller fragments for which the Z-counting polynomials are known [1,3]. In fig. 2, we give the construction of the Z-counting polynomial for the same graph G as in fig. 1, using the recurrence relation (6).



$$Q(G;x) = Q(G\text{-}e;x) + xQ(G\text{-}(e);x)$$

$$Q(G\text{-}e;x) = 1 + 5x + 6x^2 + x^3$$

$$xQ(G\text{-}(e);x) = x(1+x)(1+x) = x + 2x^2 + x^3$$

$$Q(G;x) = 1 + 6x + 8x^2 + 2x^3$$

Fig. 2. The construction of the Z-counting polynomial for a graph G, already given in fig. 1, using the recurrence relation (6).

In this note, we report the extension of the Z-counting polynomial to edge-weighted graphs. The edge-weighted graphs are of interest in various fields of science such as communication net theory [12] and chemical graph theory [2,13].

These graphs will be denoted by G^* and the edge-weights by w. In fig. 3 is given an examples of the edge-weighted graph.

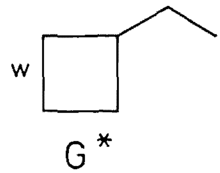
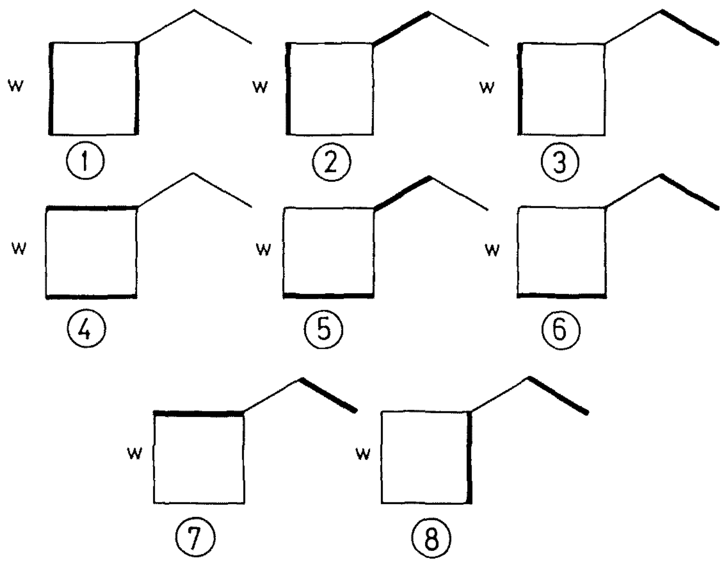


Fig. 3. An edge-weighted graph G^*.

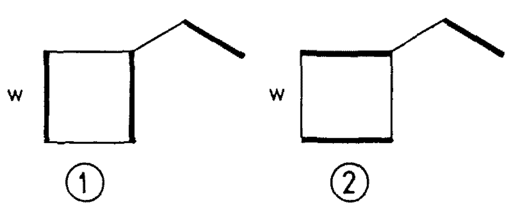
The construction of the Z-counting polynomial for edge-weighted graphs is based on a similar procedure that we developed for computing the acyclic polynomials of weighted graphs [2,5,10,13]. In this case, we had to introduce the concept of the weighted Sachs graph. For example, if we wish to compute the Z-counting polynomial for a weighted graph G^*, given in fig. 3, the following sets of Sachs graphs arise:

(i)



Subgraphs labeled by **4**–**8** are ordinary unweighted acyclic Sachs graphs, while **1**–**3** are weighted acyclic Sachs graphs. Their contribution to the coefficient $p(G^*;2)$ is $5 + 3w$.

(ii)



Subgraph labeled **1** is the weighted Sachs graph and subgraph **2** is the unweighted Sachs graph. Their contribution to the coefficient $p(G;3)$ is $1 + w$. The Z-counting polynomial of G^* is then given by

$$Q(G^*;x) = 1 + (5 + w)x + (5 + 3w)x^2 + (1 + w)x^3. \tag{7}$$

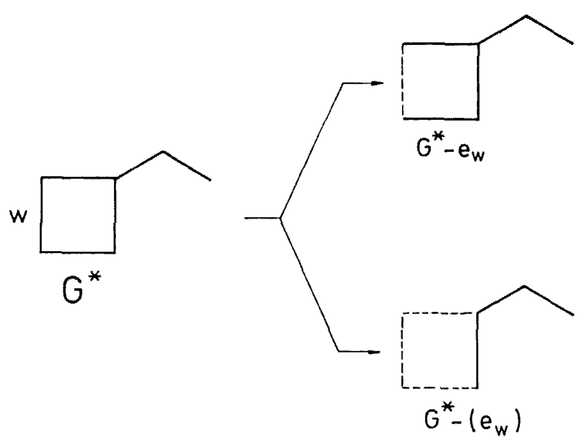
For $w = 1$, this polynomial reduces to the Z-counting polynomial of G depicting vinylcyclobutadiene (see fig. 1). If the weight $w = 0.75$ is chosen for the weighted edge in G^*, the the Z-counting polynomial from the above is given as

$$Q(G^*;x) = 1 + 5.75x + 7.25x^2 + 1.75x^3. \tag{8}$$

The Z-counting polynomial $Q(G^*;x)$ for an edge-weighted graph G^* can also be computed using recurrence relation (6), but in a modified form:

$$Q(G^*;x) = Q(G^* - e_w;x) + wx(G^* - (e_w);x), \tag{9}$$

where $G^* - e_w$ and $G^* - (e_w)$ are subgraphs obtained by removing from G^* the weighted edge e_w, and the weighted edge e_w and its incident edges, respectively. An example of using recurrence formula (9) is given in fig. 4. If there are more weighted edges



$$Q(G^*;x) = Q(G^* - e_w;x) + wx\,Q(G^* - (e_w);x)$$

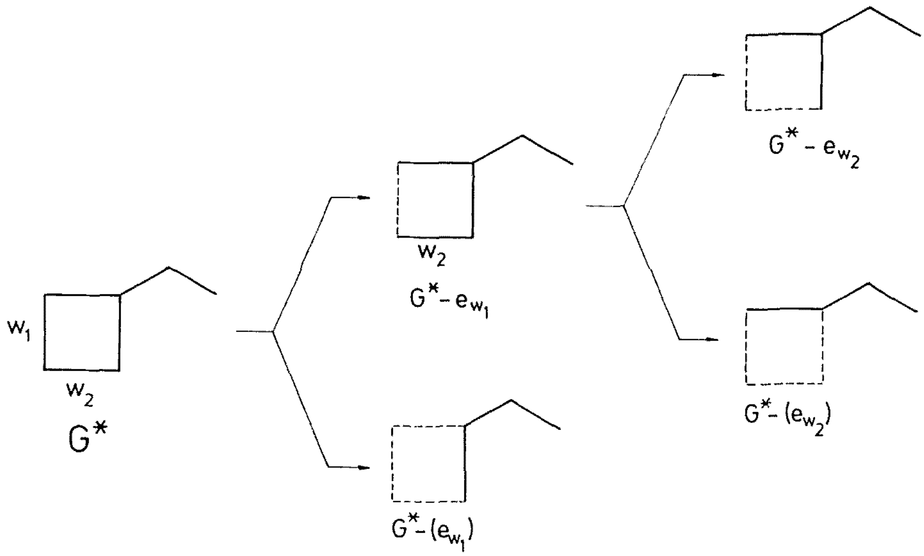
$$Q(G^* - e_w;x) = 1 + 5x + 5x^2 + x^3$$

$$wxQ(G^* - (e_w);x) = wx(1 + 3x + x^2)$$

$$= wx + 3wx^2 + wx^3$$

$$Q(G^*;x) = 1 + (5 + w)x + (5 + 3w)x^2 + (1 + w)x^3$$

Fig. 4. The construction of the Z-counting polynomial for an edge-weighted graph G^* using the recurrence relation (9).



$$Q(G^*;x) = Q(G^* - e_{w_1}) + w_1 x\, Q(G^* - (e_{w_1}))$$
$$= Q(G^* - e_{w_2}) + w_2 x Q(G^* - (e_{w_2}))$$
$$+ w_1 x Q(G^* - (e_{w_1}))$$

$$Q(G^* - e_{w_2};x) = 1 + 4x + 2x^2$$

$$w_2 x Q(G^* - (e_{w_2});x) = w_2 x(1 + 3x + x^2)$$
$$= w_2 x + 3w_2 x^2 + w_2 x^3$$

$$w_1 Q(G^* - (e_{w_1});x) = w_1 x(1 + 3x + x^2)$$
$$= w_1 x + 3w_1 x^2 + w_1 x^3$$

$$Q(G^*;x) = 1 + (4 + w_1 + w_2)x + (2 + 3w_1$$
$$+ 3w_2)x^2 + (w_1 + w_2)x^3$$

Fig. 5. A graph G^* with two weighted edges and the construction of its Z-counting polynomial.

in G^*, then the recursion (9) must be used in several steps, the number of steps being determined by the number of weighted edges. An example of a two-edge weighted graph G^* and the computation of its Z-counting polynomial is given in fig. 5.

For $w_1 = w_2$, the Z-counting polynomial given in fig. 5 reduces to

$$Q(G^*; x) = 1 + (4 + 2w)x + (2 + 6w)x^2 + 2wx^3. \quad (10)$$

The same polynomial for $w_2 = 1$ converts into the Z-counting polynomial in fig. 4.

Acknowledgement

This work was supported by the Ministry of Science, Technology and Informatics of the Republic of Croatia via Grants No. 1-07-159 and No. 1-07-165.

References

[1] H. Hosoya, Bull. Chem. Soc. Japan 44(1971)2331.
[2] N. Trinajstić, *Chemical Graph Theory*, Vol. 2 (CRC, Boca Raton, FL, 1983), p. 112.
[3] H. Hosoya, in: *Mathematics and Computational Concepts in Chemistry*, ed. N. Trinajstić (Horwood, Chichester, 1986), p. 110.
[4] I. Gutman, in: *Chemical Graph Theory: Introduction and Fundamentals*, ed. D. Bonchev and R.H. Rouvray (Abacus Press/Gordon and Breach, New York, 1991), p. 133.
[5] I. Gutman, M. Milun and N. Trinajstić, J. Amer. Chem. Soc. 99(1977)1692.
[6] O.J. Heilmann and E.H. Lieb, Phys. Rev. Lett. 24(1970)1412; Commun. Math. Phys. 22(1971)133.
[7] H. Kunz, Phys. Lett. A32(1970)311.
[8] E.J. Farrell, J. Comb. Theory B27(1979)75.
[9] C.D. Godsil and I. Gutman, J. Graph Theory 5(1981)137.
[10] N. Trinajstić, Croat. Chem. Acta 49(1977)593.
[11] A. Graovac, I. Gutman, N. Trinajstić and T. Živković, Theor. Chim. Acta 26(1972)67.
[12] W. Meyeda, *Graph Theory* (Wiley–Interscience, New York, 1972), ch. 12.
[13] N. Trinajstić, *Chemical Graph Theory*, 2nd rev. ed. (CRC, Boca Raton, FL, 1992), ch. 10.