match no. 18 pp. 49-53 1985

COMMENT ON "MATCHINGS IN LONG BENZENE CHAINS" BY E. J. FARRELL AND S. A. WAHID

Ante Graovac and Darko Babić

Institute "Rudjer Bošković"
YU-41001 Zagreb, POB 1016, Yugoslavia

Department of Physical Chemistry
Faculty of Science
YU-41001 Zagreb, POB 163, Yugoslavia

(received: November 1984)

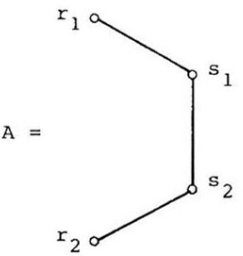
The recurrence relation of the order eight for the matching polynomial $m(L_n)$ of the long benzene chain, given by Theorem 4 in Ref. [1], has been recently derived by Farrell and Wahid. It is to be pointed out that a recurrence relation of a lower order, i.e. of the order four, can be obtained following the general procedure described in [2]. The relation reads as:

$$L_n = (w_1^4+5w_1^2w_2+4w_2^2)L_{n-1} - 2(w_1^4w_2^2+4w_1^2w_2^3+3w_2^4)L_{n-2} + (w_1^4w_2^4+3w_1^2w_2^5+4w_2^6)L_{n-3} - w_2^8L_{n-4} \quad , \quad n>3 \tag{1}$$

where $m(L_n)$ is abbreviated by L_n. The initial polynomials L_0, L_1, L_2 and L_3 are the same as in Table 1 of [1].

The graphs which exhibit one-dimensional periodicity have been already introduced in the literature [3].

They are called fasciagraphs F_n and rotagraphs R_n when they have open and closed ends, respectively. The benzene chain A_n [4] and the long benzene chain L_n [1] are the special fasciagraph and rotagraph, respectively, with the following repeating monomer graph:



The method presented in [2] is derived for the reference or acyclic polynomial, but is easily modified for the case of the closely related matching polynomial as defined by Farrell [5]. In the last case the elements of the T-matrix, which represents the base for the derivation of the recursion formulas [2], are given by:

$$T_{ij} = (w_2)^{|\sigma_j|} A^{\rho i, \sigma j} \qquad (2)$$

where $A^{\rho i, \sigma j}$ denotes the matching polynomial of a subgraph obtained by deletion of sets of vertices ρ_i and σ_j out from A. For the details the reader is referred to the Ref. [2]. Taking (2) into account, T-matrix for both the benzene chain and the long benzene chain reads as:

$$T = \begin{bmatrix} w_1^4+3w_1^2w_2+w_2^2 & w_1^3w_2+w_1w_2^2 & w_1^3w_2+w_1w_2^2 & w_1^2w_2^2 \\ w_1^3+2w_1w_2 & w_1^2w_2+w_2^2 & w_1^2w_2 & w_1w_2^2 \\ w_1^3+2w_1w_2 & w_1^2w_2 & w_1^2w_2+w_2^2 & w_1w_2^2 \\ w_1^2+w_2 & w_1w_2 & w_1w_2 & w_2^2 \end{bmatrix} \qquad (3)$$

The characteristic polynomial $\Phi(t,\lambda) = \det(\lambda I-T)$ is easily evaluated and the use of the Cayley-Hamilton theorem:

$$\Phi(T,T) = 0 \qquad (4)$$

straightforwardly yields the recurrence relations for $m(A_n)$, $m(L_n)$ and the matching polynomials of some subgraphs of A_n [2]. E.g. by equating the matrix elements in the first row and in the first column on the both sides of eqn. (4), the recurrence relation for $m(A_n)$ follows. Because of $m(L_n) = tr(T^n)$ [2], where tr denotes the trace of the matrix, the recurrence relation (1) for $m(L_n)$ is obtained by equating the trace on the both sides of eqn. (4).

The presented formalism obviously shows its advantage over the extremely tedious algebraic manipulations of [1]. Generally, it yields the recurrence relations of the order 2^{ℓ} for $m(R_n)$ and of the order lower or equal to 2^{ℓ} for $m(F_n)$, where ℓ denotes the number of linking edges between the monomer graphs. In the case of $R_n = L_n$,

ℓ equals 2, and the recurrence relation for $m(L_n)$ is obviously of the order four. In the case of $F_n = A_n$, the recurrence relation is of the order $3 < 2^2$, what has been already proved in the literature [6].

Moreover, the formalism of [2] applies generally to any F_n and R_n and its application is the matter of routine.

The above comments apply as well to the recurrence relations for the number N_d of defect-d matchings and the number γ_k of k-matchings in F_n and R_n. Especially, for the long benzene chain, instead of Theorem 5 and Theorem 8 of [1], one derives the following, lower order recurrence relations for $N_d(L_n)$ and $\gamma_k(L_n)$:

$$N_d(L_n) = (N_{d-4}+5N_{d-2}+4N_d)L_{n-1} - 2(N_{d-4}+4N_{d-2}+3N_d)L_{n-2} + \\ + (N_{d-4}+3N_{d-2}+4N_d)L_{n-3} - (N_d)L_{n-4} \quad , \quad n>3 \tag{5}$$

$$\gamma_k(L_n) = (\gamma_k+5\gamma_{k-1}+4\gamma_{k-2})L_{n-1} - 2(\gamma_{k-2}+4\gamma_{k-3}+3\gamma_{k-4})L_{n-2} + \\ + (\gamma_{k-4}+3\gamma_{k-5}+4\gamma_{k-6})L_{n-3} - (\gamma_{k-8})L_{n-4} \quad , \quad n>3 \tag{6}$$

with the same notation and with the same initial conditions as in [1]. The following convention holds: $N_d = 0$ for $d<0$ in (5), and $\gamma_k = 0$ for $k<0$ in (6). Owing to the simpler recurrence relations one is able to proceed further in the derivation of the explicit expressions for $N_d(L_n)$ and $\gamma_k(L_n)$. E.g. $N_4(L_n)$ reads as:

$$N_4(L_n) = \frac{1}{60}(n^6+20n^5+80n^4-20n^3-21n^2) \quad , \qquad n>0 \tag{7}$$

REFERENCES:

[1] E. J. Farrell and S. A. Wahid, MATCH __ (198)

[2] A. Graovac, O. E. Polansky, N. N. Tyutyulkov, Croat. Chem. Acta 56 325 (1983)

[3] O. E. Polansky and N. N. Tyutyulkov, MATCH 3 149 (1977)

[4] E. J. Farrell and S. A. Wahid, Discrete Appl. Math. 7 45 (1984)

[5] E. J. Farrell, J. Comb. Theory B27 75 (1979)

[6] I. Gutman, E. J. Farrell, S. A. Wahid, J. Comb. Inf. Syst. Sci. 8 159 (1983)