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FACTORIZATION AND RECURSION RELATIONS OF THE MATCHING AND CHARACTERISTIC POLYNOMIALS OF PERIODIC POLYMER NETWORKS

Haruo HOSOYA
Department of Chemistry, Ochanomizu University, Bunkyo-ku, Tokyo 112, Japan

Abstract

Recent developments in the analysis of mathematical structure of the matching and characteristic polynomials of linear and cyclic periodic polymer networks are surveyed, especially on the newly found efficient algorithms and techniques for deriving their recursion relations and factorization expressions. Advantages and disadvantages of these two polynomials for manipulating large networks are compared and discussed with examples. Contrary to the case of singly connected polymer networks, only a few useful mathematical properties are shown to be found for doubly connected polymer networks. Linear and cyclic fence graphs are proposed to be defined instead of the conventional definitions of the so-called Hückel and Möbius ladder graphs, so that simpler and more useful mathematical relations hold for their matching polynomials.

1. Introduction

Among the various counting polynomials, the characteristic $\mathcal{P}_G(x)$ and matching $\mathcal{M}_G(x)$ polynomials have been considered to be very important, not only in their chemical applications but also in their mathematical properties [1–3]. If one is going to analyze the chemical and physical properties of large conjugated compounds such as polycyclic benzenoid hydrocarbons and graphite, detailed knowledge of the mathematical properties of these counting polynomials for large networks is inevitably necessary, especially on their converging behavior toward infinitely large systems [4–8].

In this respect, $\mathcal{P}_G(x)$ has several advantages over $\mathcal{M}_G(x)$, such as in the computational labor and time. It is generally known that the number of procedures for obtaining the solutions of a given $\mathcal{P}_G(x)$, or for diagonalizing the secular determinant, is roughly proportional to N^4, with N being the number of the basis set, whereas for $\mathcal{M}_G(x)$ the computational time increases with $N!$, leading to the so-called combinatorial explosion. Further, for the system with periodic symmetry one can factorize $\mathcal{P}_G(x)$ into the product of the contributions of the component units by the use of the group-theoretical technique, which sometimes enables us to derive a general and closed form of $\mathcal{P}_G(x)$ [5,6].

On the contrary, general procedures for deriving the recursion relations of $\mathcal{M}_G(x)$ of a given periodic system are straightforward, while the recursion relations of $\mathcal{P}_G(x)$ have been obtained only in the luckiest cases [9]. It might be needless to say that every coefficient, i.e. the non-adjacent number $p(G, k)$, of $\mathcal{M}_G(x)$ has direct graph-theoretical and combinatorial meanings [10,11].

The crucial computational disadvantages of $\mathcal{M}_G(x)$ come from the fact that owing to its combinatorial definition there is no known general and straightforward algorithm for obtaining a matrix expression to give $\mathcal{M}_G(x)$ for a polycyclic graph. In other words, for a given polycyclic graph G there is no guarantee for the existence of the associated graph whose characteristic polynomial exactly gives the target $\mathcal{M}_G(x)$ [12–14]. For several selected polycyclic graphs, the present author recently derived an algorithm for finding a set of associated graphs $\{H_i\}$ with imaginary weights, so that the weighted mean of the $\mathcal{P}_{H_i}(x)$'s gives the $\mathcal{M}_G(x)$ [15,16]. Graovac et al. tried to explore the factorization of $\mathcal{M}_G(x)$ for periodic polymer networks and were able to derive a useful algorithm for a singly connected polymer network [17,18]. However, for more complicated cases, even for a doubly connected polymer network, almost nothing has been reported on the factorization of $\mathcal{M}_G(x)$. Polansky tried to analyze the relation between the roots of the characteristic and matching polynomials of Hückel- and Möbius-type polyacenes [19]. The purpose of the present paper is to survey the state-of-the-art and the possibility of a breakthrough of this problem.

2. Definitions of periodic graphs and matching polynomial

Let the characteristic and matching polynomials of a monomer unit M be denoted as $\underline{\mathcal{M}}$ and $\mathcal{M}$, respectively. The definition of the matching polynomial is essentially the same as the Z-counting polynomial [10,11] by using the non-adjacent number $p(G, k)$ [20–23]. Consider linear and cyclic n-mers, M_n and ${}^0M_n$, respectively, by joining consecutively the atoms r and s ($\neq r$) of the neighboring units as in fig. 1. Sometimes, the graphs M_n and ${}^0M_n$ are called, respectively, fascia-

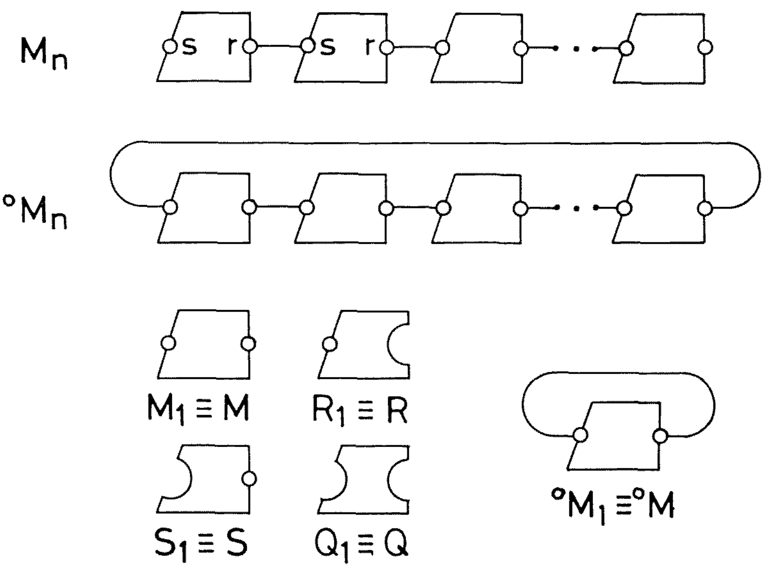


Fig. 1. Linear and cyclic polymers M_n and ${}^0M_n$ composed of monomer units M, together with its subgraphs R, S and Q.

and rotagraphs [24]. Let the polynomials $\mathcal{M}_1$ be simply denoted as $\mathcal{M}$. The subgraphs R, S, and Q of M are defined, respectively, as $M \ominus r$, $M \ominus s$, and $M \ominus (r, s)$ [25]. The notation $M \ominus r$ means the subgraph of M obtained by deletion of r and all the lines adjacent to r.

3. New techniques for obtaining the recursion relations of counting polynomials

Recently, various techniques for obtaining the recursion relations of $\mathcal{P}_G(x)$ and $\mathcal{M}_G(x)$ have been proposed, such as the operator technique [9], transfer matrix [26], and pruning method [27]. Here, the former two methods will be explained.

3.1. OPERATOR TECHNIQUE

Define the step-up operator $\mathbb{O}$ to shift the counting polynomial $\mathcal{F}_n$ up to $\mathcal{F}_{n+1}$ as [9]

$$\mathbb{O}\,\mathcal{F}_n = \mathcal{F}_{n+1}. \tag{1}$$

For the time being, let us consider that $\mathcal{F}_n$ is a matching polynomial. Although there is no guarantee for all the family of polynomials related to $\mathcal{M}_n$, namely, $\mathcal{R}_n$, $\mathcal{S}_n$, and $\mathcal{Q}_n$, to obey the same operator $\mathbb{O}$, let us dare to assume eq. (1) for all of them. Then, as will be clear from fig. 2, we obtain the following pair of recursion relations for $\mathcal{M}_n$ and $\mathcal{S}_n$:

$$\begin{cases} \mathcal{M}_n = \mathcal{M}\,\mathcal{M}_{n-1} - \mathcal{R}\mathcal{S}_{n-1}, \\ \mathcal{S}_n = \mathcal{S}\,\mathcal{M}_{n-1} - \mathcal{Q}\mathcal{S}_{n-1}, \end{cases} \tag{2}$$

which can be transformed into the operator expression as

$$\begin{cases} (\mathbb{O} - \mathcal{M})\mathcal{M}_n + \mathcal{R}\mathcal{S}_n = 0, \\ -\mathcal{S}\,\mathcal{M}_n + (\mathbb{O} + \mathcal{Q})\mathcal{S}_n = 0. \end{cases} \tag{3}$$

In order for $\mathcal{M}_n$ and $\mathcal{S}_n$ to be non-trivial, the following coefficient determinant derived from eq. (3) should be fulfilled:

$$\Delta = \begin{vmatrix} \mathbb{O} - \mathcal{M} & \mathcal{R} \\ -\mathcal{S} & \mathbb{O} + \mathcal{Q} \end{vmatrix}$$

$$= \mathbb{O}^2 - (\mathcal{M} - \mathcal{Q})\mathbb{O} + (\mathcal{R}\mathcal{S} - \mathcal{M}\mathcal{Q}) = 0. \tag{4}$$

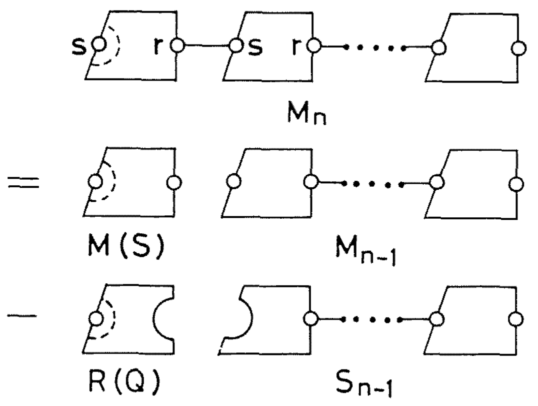


Fig. 2. Recursion relation (2) for the matching and characteristic polynomials of M_n and S_n (dotted).

Then, application of this operator polynomial Δ to $\mathcal{M}_{n-2}$ gives the desired recursion relation

$$\mathcal{M}_n = (\mathcal{M} - \mathcal{Q})\,\mathcal{M}_{n-1} - (\mathcal{R}\mathcal{S} - \mathcal{M}\,\mathcal{Q})\,\mathcal{M}_{n-2}, \tag{5}$$

which is shown to be fulfilled also by $\mathcal{R}_n$, $\mathcal{S}_n$, and $\mathcal{Q}_n$.

Let us define the canonical operator polynomial $\mathcal{F}(\mathbb{O}, x)$ to be the operator polynomial of the least order for describing the recursion relation of the counting polynomial of a given series of graphs. In this case, the coefficient determinant Δ is found to be identical to $\mathcal{F}(\mathbb{O}, x)$.

For a later purpose, let us rewrite eq. (5) as

$$\mathcal{M}_n = \mathcal{A}\,\mathcal{M}_{n-1} - \mathcal{B}\,\mathcal{M}_{n-2}, \tag{6}$$

with $\mathcal{A} = \mathcal{M} - \mathcal{Q}$ and $\mathcal{B} = \mathcal{R}\mathcal{S} - \mathcal{M}\,\mathcal{Q}$.

Note that $\mathcal{A}$ is nothing but the matching polynomial of the cyclic monomer of ${}^0M_n$, namely, $\mathcal{A} = {}^0\mathcal{M}_1 = {}^0\mathcal{M}$. Further, ${}^0\mathcal{M}_n$ is also shown to obey the same recursion relation as $\mathcal{M}_n$,

$$\begin{aligned}
{}^0\mathcal{M}_n &= \mathcal{M}_n - \mathcal{Q}_n \\
&= (\mathcal{A}\,\mathcal{M}_{n-1} - \mathcal{B}\,\mathcal{M}_{n-2}) - (\mathcal{R}\mathcal{S}_{n-1} - \mathcal{Q}\mathcal{Q}_{n-1}) \\
&= \mathcal{A}\,\mathcal{M}_{n-1} - \mathcal{B}\,\mathcal{M}_{n-2} - \mathcal{R}(\mathcal{M}\mathcal{S}_{n-2} - \mathcal{S}\,\mathcal{Q}_{n-2}) + \mathcal{Q}\mathcal{Q}_{n-1} \\
&= \mathcal{A}\,\mathcal{M}_{n-1} - \mathcal{B}\,\mathcal{M}_{n-2} - \mathcal{M}(\mathcal{Q}_{n-1} + \mathcal{Q}\mathcal{Q}_{n-2}) + \mathcal{R}\mathcal{S}\,\mathcal{Q}_{n-2} + \mathcal{Q}\mathcal{Q}_{n-1} \\
&= \mathcal{A}\,{}^0\mathcal{M}_{n-1} - \mathcal{B}\,{}^0\mathcal{M}_{n-2},
\end{aligned} \tag{7}$$

with the factors $\mathcal{A}$ and $\mathcal{B}$ common to eq. (6). We can formulate this relation as

$$\mathcal{F}(\mathbb{O}, x) = {}^0\mathcal{F}(\mathbb{O}, x) = \mathbb{O}^2 - (\mathcal{M} - \mathcal{Q})\mathbb{O} + (\mathcal{R}\mathcal{S} - \mathcal{M}\mathcal{Q}). \tag{8}$$

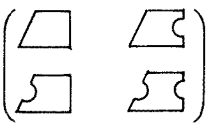
3.2. TRANSFER MATRIX

In this case, eq. (2) can be expressed in matrix form:

$$\begin{pmatrix} \mathcal{M}_n \\ \mathcal{S}_n \end{pmatrix} = \begin{pmatrix} \mathcal{M} & -\mathcal{R} \\ \mathcal{S} & -\mathcal{Q} \end{pmatrix} \begin{pmatrix} \mathcal{M}_{n-1} \\ \mathcal{S}_{n-1} \end{pmatrix}. \tag{9}$$

After defining the transfer matrix $\mathbb{T}$ as

$$\mathbb{T} = \begin{pmatrix} \mathcal{M} & -\mathcal{R} \\ \mathcal{S} & -\mathcal{Q} \end{pmatrix} =$$



(10)

followed by its successive application, one obtains

$$\begin{pmatrix} \mathcal{M}_n \\ \mathcal{S}_n \end{pmatrix} = \mathbb{T} \begin{pmatrix} \mathcal{M}_{n-1} \\ \mathcal{S}_{n-1} \end{pmatrix} = \mathbb{T}^n \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{11}$$

Note that all the elements of $\mathbb{T}^n$ correspond to the matching polynomials of the nth entries of the series of graphs relevant to M_n as

$$\mathbb{T}^n = \begin{pmatrix} \mathcal{M}_n & -\mathcal{R}_n \\ \mathcal{S}_n & -\mathcal{Q}_n \end{pmatrix}. \tag{12}$$

Then, as has been pointed out by Graovac and Babic [28,29], the matching polynomial of the cyclic polymer ${}^0M_n$ can be expressed as the trace of $\mathbb{T}^n$,

$${}^0\mathcal{M}_n = \mathcal{M}_n - \mathcal{Q}_n = \mathrm{Tr}(\mathbb{T}^n). \tag{13}$$

It is interesting to observe that the operator polynomial Δ (eq. (4)) obtained from the operator technique is equal to the determinant of the transfer matrix $\mathbb{T}$, namely,

$$\Delta = \det(\mathbb{O}\boldsymbol{E} - \mathbb{T}), \tag{14}$$

with the unit matrix $\boldsymbol{E}$ of order 2.

Graovac and Babic [28,29] proved that the matching polynomial of a singly connected periodic polymer ${}^0M_n$ can be factorized in terms of the polynomials $\mathcal{A}$ and $\mathcal{B}$ used in the recursion relations (eqs. (6) and (7)) for $\mathcal{M}_n$ and ${}^{0}\mathcal{M}_n$ as

$${}^{0}\mathcal{M}_n = \prod_{k=1}^{n} \left\{ A - 2\sqrt{B}\cos\frac{(2k-1)\pi}{2n} \right\}. \tag{15}$$

They have pointed out that this relation is in full analogy with that for the characteristic polynomial

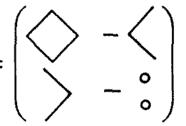
$${}^{0}\underline{\mathcal{M}}_n = \prod_{k=1}^{n} \left\{ A - 2\sqrt{B}\cos\frac{2k\pi}{n} \right\}. \tag{16}$$

Namely, all the discussions between eqs. (1) and (14) except eqs. (7), (8), and (13) can also be applied to the characteristic polynomial.

4. Examples of singly connected polymers

Let us expose several examples showing various recursion and factorization properties. In table 1, the matching polynomials of the linear and cyclic periodic polymers (poly-p-cyclobutadienylene) composed of square rings are given. In this case, M is a square graph, R $(=S)$ is a path graph composed of three points, and Q is a pair of disjoint points. Then, the transfer matrix becomes

$$\mathbb{T} = \begin{pmatrix} x^4 - 4x^2 + 2 & -(x^3 - 2x) \\ x^3 - 2x & -x^2 \end{pmatrix} = \tag{17}$$



By using this transfer matrix, the matching polynomials of the linear and cyclic polymers can straightforwardly be obtained from eqs. (11) and (13).

The canonical operator polynomial for describing commonly the recursion relations of $\mathcal{M}_n$, $\mathcal{R}_n$, $\mathcal{S}_n$, and $\mathcal{Q}_n$ is obtained as

$$\mathcal{F}(\mathbb{O}, x) = \det(\mathbb{O}\boldsymbol{E} - \mathbb{T}) = \mathbb{O}^2 - (x^4 - 5x^2 + 2)\mathbb{O} + 2x^2. \tag{18}$$

Then, the recursion relations of both polymers are written down as

$$\mathcal{M}_n(x) = (x^4 - 5x^2 + 2)\,\mathcal{M}_{n-1}(x) - 2x^2\,\mathcal{M}_{n-2}(x), \tag{19}$$

$${}^{0}\mathcal{M}_n(x) = (x^4 - 5x^2 + 2)\,{}^{0}\mathcal{M}_{n-1}(x) - 2x^2\,{}^{0}\mathcal{M}_{n-2}(x), \tag{20}$$

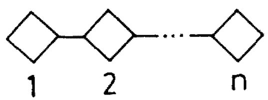
as a special case of eqs. (6) and (7) with

Table 1

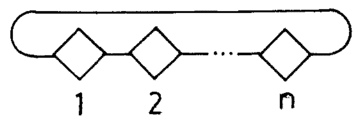
Matching polynomials of linear and cyclic poly-p-cyclobutadienylene graphs and the related graphs

n	0[a]	1	2	3
${}^{0}\mathcal{M}_n$	2	x^4-5x^2+2	$x^8-10x^6+29x^4-24x^2+4$	$x^{12}-15x^{10}+81x^8-191x^6+192x^4-72x^2+8$
$\mathcal{M}_n$	1	x^4-4x^2+2	$x^8-9x^6+24x^4-20x^2+4$	$x^{12}-14x^{10}+71x^8-160x^6+160x^4-64x^2+8$
$\left.\begin{matrix}\mathcal{R}_n\\ =\mathcal{S}_n\end{matrix}\right\}$	0	x^3-2x	$x^7-7x^5+12x^3-4x$	$x^{11}-12x^9+49x^7-80x^5+48x^3-8x$
$\mathcal{Q}_n$	-1	x^2	$x^6-5x^4+4x^2$	$x^{10}-10x^8+31x^6-32x^4+8x^2$

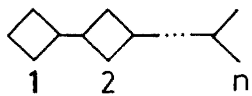
M_n :



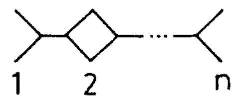
${}^{0}M_n$:



R_n, S_n :



Q_n :



[a]The polynomials for the entries with $n = 0$ are assigned so that the recursion relations in table 3, eqs. (2) and (5) hold for all the entries with $n \geq 0$.

$$\mathcal{A} = x^4 - 5x^2 + 2 \quad \text{and} \quad \mathcal{B} = 2x^2. \tag{21}$$

Namely, the relation (8) is shown to hold in this case.

Although ${}^0\mathcal{M}_n$ can be factored out according to eq. (15) to be

$${}^0\mathcal{M}_n = \prod_{k=1}^{n} \left\{ (x^4 - 5x^2 + 2) - 2\sqrt{2}x \cos \frac{(2k-1)\pi}{2n} \right\}, \tag{22}$$

$\mathcal{M}_n$ cannot be factored out.

The characteristic polynomial of the cyclic graph ${}^0M_n$ is also obtained as (see eq. (16) and table 2)

$${}^0\underline{\mathcal{M}}_n = \prod_{k=1}^{n} \left\{ (x^4 - 5x^2) - 4x \cos \frac{2k\pi}{n} \right\}. \tag{23}$$

Table 2

Characteristic polynomials of linear, cyclic poly-p-cyclobutadienylenes and the related graphs[a)]

n	0[b)]	1	2	3
${}^0\underline{\mathcal{M}}_n$	0	$x^4 - 5x^2 - 4x$	$x^8 - 10x^6 + 25x^4 - 16x^2$	$x^{12} - 15x^{10} + 75x^8 - 137x^6 + 60x^4 - 16x^3$
$\underline{\mathcal{M}}_n$	1	$x^4 - 4x^2$	$x^8 - 9x^6 + 20x^4 - 4x^2$	$x^{12} - 14x^{10} + 65x^8 - 108x^6 + 36x^4$
$\left.\begin{matrix}\underline{\mathcal{R}}_n \\ = \underline{\mathcal{S}}_n\end{matrix}\right\}$	0	$x^3 - 2x$	$x^7 - 7x^5 + 10x^3$	$x^{11} - 12x^9 + 45x^7 - 54x^5 + 8x^3$
$\underline{\mathcal{Q}}_n$	1	x^2	$x^6 - 5x^4 + 4x^2$	$x^{10} - 10x^8 + 29x^6 - 24x^4$

[a)]Graphs are given in table 1. [b)]See footnote a) in table 1.

It is to be noted that the factorization of the characteristic polynomial for the *cyclic* polymer is performed in terms of the recursion relation for the *linear* polymer,

$$\underline{\mathcal{M}}_n(x) = (x^4 - 5x^2)\, \underline{\mathcal{M}}_{n-1}(x) - 4x^2\, \underline{\mathcal{M}}_{n-2}(x). \tag{24}$$

Actually, the characteristic polynomial of the cyclic polymer ${}^0M_n$ is found to recur as

$$\begin{aligned} {}^0\underline{\mathcal{M}}_n(x) &= (x^4 - 5x^2 + 2x)\, {}^0\underline{\mathcal{M}}_{n-1}(x) \\ &\quad - (2x^5 - 10x^3 + 4x^2)\, {}^0\underline{\mathcal{M}}_{n-2}(x) + 8x^3\, {}^0\underline{\mathcal{M}}_{n-3}(x). \end{aligned} \tag{25}$$

The close relationship among the recursion relations (19), (20), (24), and (25) is easily seen by using the operator polynomials as summarized in table 3. Namely, eq. (25) is found to contain eq. (24) if they are expressed in terms of the canonical operator polynomial.

Table 3

Recursion relations and factorization of the matching and characteristic polynomials of linear and cyclic poly-p-cyclobutadienylenes

Polynomial	Recursion relation	Factorization
$\mathcal{M}_n$ [a]	$O^2 - (x^4 - 5x^2 + 2)O + 2x^2$	–
$\underline{\mathcal{M}}_n$ [a]	$O^2 - (x^4 - 5x^2)O + 4x^2$	–
${}^0\mathcal{M}_n$	$O^2 - (x^4 - 5x^2 + 2)O + 2x^2$	$\prod_{k=1}^{n}\left\{(x^4 - 5x^2 + 2) - 2\sqrt{2}x\cos\frac{(2k-1)\pi}{2n}\right\}$
${}^0\underline{\mathcal{M}}_n$	$(O - 2x)[O^2 - (x^4 - 5x^2)O + 4x^2]$ $= O^3 - (x^4 - 5x^2 + 2x)O^2$ $+ (2x^5 - 10x^3 + 4x^2)O - 8x^3$	$\prod_{k=1}^{n}\left\{(x^4 - 5x^2) - 4x\cos\frac{2k\pi}{n}\right\}$

As another example of mathematically interesting relations among the recursion relations and factorization of $\mathcal{P}_G(x)$ and $\mathcal{M}_G(x)$, the results of the linear and cyclic comb graphs are summarized in tables 4 and 5. In this case, the joint atoms r and s coincide and all the discussions between eqs. (1) and (16) are found to be valid just by putting $\mathcal{R} = \mathcal{S} = x$, $\mathcal{R}_n = x\mathcal{M}_{n-1}$, and $\mathcal{Q} = 0$.

Then, the following transfer matrix expression for $\mathcal{M}_n$ is obtained:

$$\begin{pmatrix} \mathcal{M}_n \\ \mathcal{S}_n \end{pmatrix} = \begin{pmatrix} x^2 - 1 & -x \\ x & 0 \end{pmatrix} \begin{pmatrix} \mathcal{M}_{n-1} \\ \mathcal{S}_{n-1} \end{pmatrix} = \mathbb{T}^n \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Similarly, for the other series of polynomials we can obtain the transfer matrix expressions as follows:

$$\begin{pmatrix} {}^0\mathcal{M}_n \\ \mathcal{M}_n \\ \mathcal{S}_n \end{pmatrix} = \begin{pmatrix} 0 & x^2 - 1 & -2x \\ 0 & x^2 - 1 & -x \\ 0 & x & 0 \end{pmatrix} \begin{pmatrix} {}^0\mathcal{M}_{n-1} \\ \mathcal{M}_{n-1} \\ \mathcal{S}_{n-1} \end{pmatrix} = {}^0\mathbb{T}^n \begin{pmatrix} 2^{\star} \\ 1 \\ 0 \end{pmatrix},$$

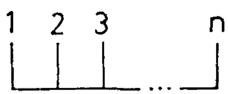
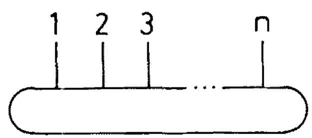
$$\begin{pmatrix} {}^0\underline{\mathcal{M}}_n \\ \underline{\mathcal{M}}_n \\ \underline{\mathcal{S}}_n \end{pmatrix} = \begin{pmatrix} x & x^2 - 2x - 1 & x^2 - 2x - 1 \\ 0 & x^2 - 1 & -x \\ 0 & x & 0 \end{pmatrix} \begin{pmatrix} {}^0\underline{\mathcal{M}}_{n-1} \\ \underline{\mathcal{M}}_{n-1} \\ \underline{\mathcal{S}}_{n-1} \end{pmatrix} = {}^0\underline{\mathbb{T}}^n \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

*Although this value has nothing to do with the derivation of ${}^0\mathcal{M}_n$ with $n \geq 1$, the ${}^0\mathcal{M}_n$ value is given in the initial vector for the sake of consistency as to the recursion relation given in table 5.

Table 4

Matching and characteristic polynomials of linear and cyclic comb graphs[a]

n	$\mathcal{M}_n(x) \equiv \underline{\mathcal{M}}_n(x)$	${}^0\mathcal{M}_n(x)$	${}^0\underline{\mathcal{M}}_n(x)$
0	1[b]	2[b]	0[b]
1	$x^2 - 1$	$x^2 - 1$	$x^2 - 2x - 1$[b]
2	$x^4 - 3x^2 + 1$	$x^4 - 4x^2 + 1$	$x^4 - 6x^2 + 1$
3	$x^6 - 5x^4 + 5x^2 - 1$	$x^6 - 6x^4 + 6x^2 - 1$	$x^6 - 6x^4 - 2x^3 + 6x^2 - 1$
4	$x^8 - 7x^6 + 13x^4 - 7x^2 + 1$	$x^8 - 8x^6 + 16x^4 - 8x^2 + 1$	$x^8 - 8x^6 + 14x^4 - 8x^2 + 1$
5	$x^{10} - 9x^8 \pm 25x^6 - 25x^4 + 9x^2 - 1$	$x^{10} - 10x^8 + 30x^6 - 30x^4 + 10x^2 - 1$	$x^{10} - 10x^8 + 30x^6 - 2x^5 - 30x^4 + 10x^2 - 1$

[a] M_n:  . ${}^0M_n$:  . ${}^0M_1$: . ${}^0M_2$:  .

[b] The recursion relations for these polynomials in table 5 hold for all the entries above $n = 0$ by assigning the initial conditions at these values.

Table 5

Recursion relations and factorization of the matching and characteristic polynomials of linear and cyclic comb graphs

Polynomial	Recursion relation $\mathcal{F}(\mathbb{O}, x)$	Factorization
$\mathcal{M}_n$	$\mathcal{F} = \mathbb{O}^2 - (x^2 - 1)\mathbb{O} + x^2$	$\prod_{k=1}^{n} \left\{ (x^2 - 1) - 2x \cos \frac{k\pi}{n+1} \right\}$
$\underline{\mathcal{M}}_n$	$\underline{\mathcal{F}} = \mathbb{O}^2 - (x^2 - 1)\mathbb{O} + x^2$	$\prod_{k=1}^{n} \left\{ (x^2 - 1) - 2x \cos \frac{k\pi}{n+1} \right\}$
${}^0\mathcal{M}_n$	${}^0\mathcal{F} = \mathbb{O}^2 - (x^2 - 1)\mathbb{O} + x^2$	$\prod_{k=1}^{n} \left\{ (x^2 - 1) - 2x \cos \frac{(2k-1)\pi}{2n} \right\}$
${}^0\underline{\mathcal{M}}_n$	${}^0\underline{\mathcal{F}} = (\mathbb{O} - x)\{\mathbb{O}^2 - (x^2 - 1)\mathbb{O} + x^2\}$ $= \mathbb{O}^3 - (x^2 + x - 1)\mathbb{O}^2 + (x^3 + x^2 - x)\mathbb{O} - x^3$	$\prod_{k=1}^{n} \left\{ (x^2 - 1) - 2x \cos \frac{2k\pi}{n} \right\}$

Due to its simpler structure, both the matching and characteristic polynomials of the linear polymer are equivalent and thus have the same mathematical properties, as $\mathcal{F}(\mathbb{O}, x) = \underline{\mathcal{F}}(\mathbb{O}, x)$ and $\mathbb{T} = \underline{\mathbb{T}}$. The matching polynomial of the cyclic polymer recurs in just the same way as the linear polymer ${}^0\mathcal{F}(\mathbb{O}, x) = \mathcal{F}(\mathbb{O}, x)$. Further, it is interesting to observe that the relation among the arguments of the cosine functions give the zeros of the family of the four polynomials in table 5.

5. Doubly connected polymer networks

We have been studying the mathematical structure of the characteristic and matching polynomials of a large number of periodic networks, both of linear and cyclic structure. Although we have not yet obtained the mathematical proofs for all of the findings, several important conjectures for these polynomials were obtained. Here, the following findings, in particular for the doubly connected polymers, are given without any proof, the details of which will be given in a future paper.

According to the standard recipe, one can factorize the characteristic polynomial ${}^0\underline{\mathcal{M}}_n(x)$ of a cyclic periodic polymer with a pair of bridge bonds connecting every pair of neighboring units (M's) [5,6]. Then, ${}^0\underline{\mathcal{M}}_n(x)$ can formally be expressed as the product of the factor f_k as

$$ {}^0\underline{\mathcal{M}}_n(x) = \prod_{k=1}^{n} f_k , $$

with

$$f_k = A - 2B\cos k\theta - 4C\cos^2 k\theta,$$

where A, B, and C are polynomials in terms of x. The $\cos k\theta$ comes from the phase factor of $\exp(\mathrm{i}k\pi/n) = \exp(\mathrm{i}k\theta)$ assigned to a bridge bond in the off-diagonal element of the determinant of f_k.

We have found empirically that the operator polynomial for the recursion formula of the characteristic polynomial $\underline{\mathcal{M}}_n$ of a doubly connected linear polymer M_n has either of the following three forms:

$$\underline{\mathcal{F}}(\mathbb{O}, x) = \begin{cases} (\mathbb{O}^6 - 1) \ - A(\mathbb{O}^5 - \mathbb{O}) + (2A + B^2 - 3C)(\mathbb{O}^4 - \mathbb{O}^2) & \mathrm{I} \\ (\mathbb{O}^5 + 1) - (A - 1)(\mathbb{O}^4 + \mathbb{O}) + (A + B^2 - 3C + 1)(\mathbb{O}^3 + \mathbb{O}^2), & \mathrm{II} \\ (\mathbb{O}^4 + 1) - A(\mathbb{O}^3 + \mathbb{O}) + (2A + B^2 - 3C + 1)\mathbb{O}^2. & \mathrm{III} \end{cases}$$

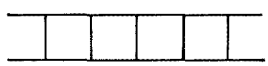
Note that

$$\mathrm{I} = (\mathbb{O} - 1)\,\mathrm{II} = (\mathbb{O}^2 - 1)\mathrm{III}.$$

The canonical operator polynomial ${}^0\underline{\mathcal{F}}(\mathrm{O}, x)$ for the recursion relation of the characteristic polynomial ${}^0\underline{\mathcal{M}}_n(x)$ of the corresponding cyclic polymer ${}^0M_n$ is not yet obtained, but we can conjecture that ${}^0\underline{\mathcal{F}}(\mathbb{O}, x)$ should contain $\underline{\mathcal{F}}(\mathbb{O}, x)$ as the principal factor, i.e.

$${}^0\underline{\mathcal{F}}(\mathbb{O}, x) \supset \underline{\mathcal{F}}(\mathbb{O}, x). \tag{26}$$

As the simplest case, one can choose an ethylene skeleton as the unit to give the following polymer network:

 ,

a single row of polyominoes, or a ladder graph [30]. If one is going to extend this network to a cyclic structure, there are two possibilities available, namely, a Hückel ladder or a Möbius ladder [31]. However, our move is to choose a third possibility, namely, to define the cyclic fence graph ${}^0F_n$ [32], which is bipartite, as in fig. 3. One may call the linear ladder the linear fence graph. By choosing this way, one can obtain simpler expressions, not only for the recursion relations but also for the transfer matrix for the matching polynomials of the series of relevant graphs. Here, only the essential results will be given. In table 6, the matching polynomials of the relevant series of graphs, together with the canonical operator polynomial for representing the recursion relations, are given.

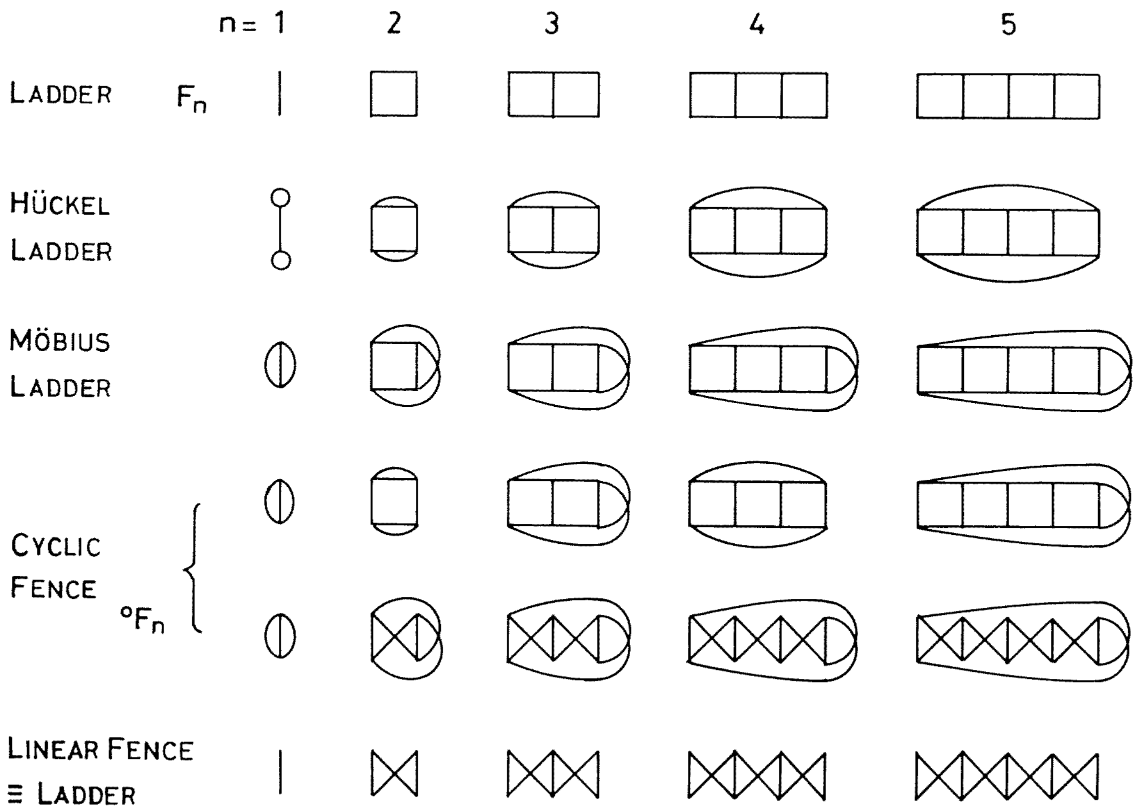
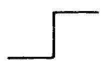
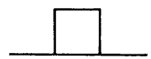
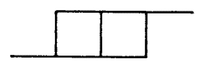
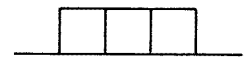
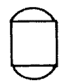
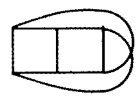
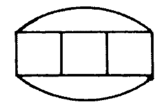
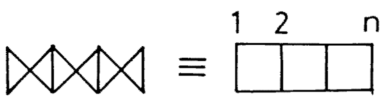
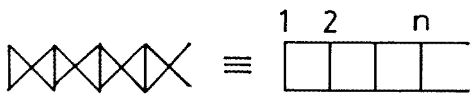
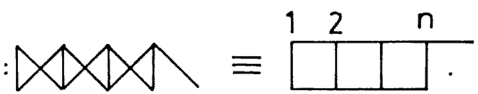


Fig. 3. Lower members of the ladder, Hückel ladder, Möbius ladder, and linear and cyclic fence graphs.

Table 6

Matching polynomials of the cyclic fence graph and related graphs

n	0	1	2	3	4
$\mathcal{A}_n$ [a]	1	x^2-1	x^4-4x^2+2	$x^6-7x^4+11x^2-3$	$x^8-10x^6+29x^4-26x^2+5$
$\mathcal{B}_n$ [a]	x^2	x^4-3x^2+1	$x^6-6x^4+7x^2-1$	$x^8-9x^6+22x^4-15x^2+2$	$x^{10}-12x^8+46x^6-65x^4+30x^2-3$
$\mathcal{C}_n$ [a]	x	x^3-2x	x^5-5x^3+4x	$x^7-8x^5+16x^3-7x$	$x^9-11x^7+37x^5-42x^3+12x$
$\mathcal{D}_n$	x^2-1	x^4-3x^2+1	$x^6-6x^4+7x^2-1$	$x^8-9x^6+22x^4-14x^2+1$	$x^{10}-12x^8+46x^6-64x^4+26x^2-1$
					
${}^0\mathcal{F}_n$	4 [b]	x^2-3	x^4-6x^2+5	$x^6-9x^4+18x^2-6$	$x^8-12x^6+42x^4-44x^2+9$
	?				

[a] $\mathcal{A}_n$:  . $\mathcal{B}_n$:  . $\mathcal{C}_n$:  .

[b] Although no corresponding graph exists, the following recursion relation holds for $n \geq 4$ by assigning this value to ${}^0\mathcal{F}_0$. Recursion relations $\mathcal{A}_n$, $\mathcal{B}_n$, $\mathcal{C}_n$: $\mathbb{O}^3-(x^2-2)\mathbb{O}^2+x^2\mathbb{O}-1=\mathcal{F}(\mathbb{O},x)$. $\mathcal{D}_n$, $\mathcal{F}_n$: $\mathbb{O}^4-(x^2-3)\mathbb{O}^3+2\,\mathbb{O}^2+(x^2-1)\mathbb{O}-1=(\mathbb{O}+1)\{\mathbb{O}^3-(x^2-2)\mathbb{O}^2+x^2\mathbb{O}-1)$ $={}^0\mathcal{F}(\mathbb{O},x)$.

The transfer matrix was obtained as

$$\begin{pmatrix} {}^0\mathcal{F}_n \\ \mathcal{A}_n \\ \mathcal{B}_n \\ \mathcal{C}_n \\ \mathcal{D}_n \end{pmatrix} = \begin{pmatrix} 0 & x^2-1 & 2 & -4x & 2 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -(x^2-1) & x^2 & -2x & 0 \\ 0 & -x & x & -1 & 0 \\ 0 & -x^2 & x^2 & -x & -1 \end{pmatrix} \begin{pmatrix} {}^0\mathcal{F}_{n-1} \\ \mathcal{A}_{n-1} \\ \mathcal{B}_{n-1} \\ \mathcal{C}_{n-1} \\ \mathcal{D}_{n-1} \end{pmatrix} = {}^0\mathbb{T}^n \begin{pmatrix} 0 \\ 1 \\ x^2 \\ x \\ x^2-1 \end{pmatrix}.$$

This transfer matrix ${}^0\mathbb{T}$ for the matching polynomial of the cyclic fence graph was found to contain that of the linear ladder graph as

$$\begin{pmatrix} \mathcal{A}_n \\ \mathcal{B}_n \\ \mathcal{C}_n \end{pmatrix} = \begin{pmatrix} -1 & 1 & 0 \\ -(x^2-1) & x^2 & -2x \\ -x & x & -1 \end{pmatrix} \begin{pmatrix} \mathcal{A}_{n-1} \\ \mathcal{B}_{n-1} \\ \mathcal{C}_{n-1} \end{pmatrix} = \mathbb{T}^n \begin{pmatrix} 1 \\ x^2 \\ x \end{pmatrix}.$$

Further, notice that

$$\det(\mathbb{O}\,\boldsymbol{E} - \mathbb{T}) = \mathcal{F}(\mathbb{O}, x) = \mathbb{O}^3 - (x^2-2)\mathbb{O}^2 + x^2\mathbb{O} - 1,$$

$$\det(\mathbb{O}\,\boldsymbol{E} - {}^0\mathbb{T}) = \mathbb{O}\;{}^0\mathcal{F}(\mathbb{O}, x) = \mathbb{O}(\mathbb{O} + 1)\;\mathcal{F}(\mathbb{O}, x),$$

where $\mathcal{F}$ and ${}^0\mathcal{F}$ are the canonical operator polynomials for the linear and cyclic fence graphs, respectively, as given in table 6.

The characteristic polynomial of the cyclic fence graph is straightforwardly factorized as

$${}^0\underline{\mathcal{F}}_n(x) = \prod_{k=1}^{n} f_k,$$

$$f_k = x^2 - \left(1 + 2\cos\frac{2k\pi}{n}\right)^2.$$

However, we have not yet succeeded in obtaining the recursion relation of the characteristic polynomial of this graph.

Another target for us to aim at for this cyclic fence graph is to factorize out the matching polynomial. The zeros of the matching polynomials of the cyclic fence graphs are found to form a well-behaved pattern as shown in fig. 4, whereas neither of the corresponding figures for the Hückel and Möbius ladder graphs shows a smooth pattern. This fact is tempting us to find a factorization of ${}^0\mathcal{F}_n(x)$.

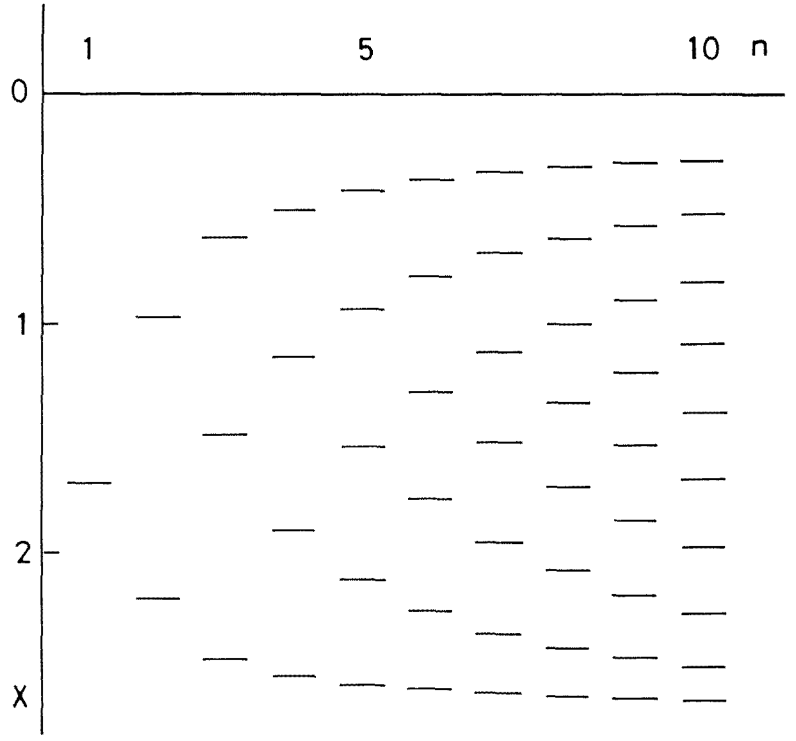


Fig. 4. Distribution of the zeros $\{x > 0 \mid {}^{0}\mathcal{F}_n(x) = 0\}$ of the matching polynomial ${}^{0}\mathcal{F}_n$ of the cyclic fence graphs.

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