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Exact dimer statistics and characteristic polynomials of cacti lattices*

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Summary. The pruning method developed earlier by one of the authors (K.B.) combined with the operator method is shown to yield powerful recursive relations for generating functions for dimer statistics and characteristic polynomials of cacti graphs and cacti lattices. The method developed is applied to linear cacti, Bethe cacti of any length containing rings of any size, and cyclic cacti of any length and size. It is shown that exact dimer statistics can be done on any cactus lattice.

Key words: Cacti lattices — Dimer statistics — Graph theory — Characteristic polynomials

1. Introduction

A fascinating problem in statistical physics which remains unsolved, in general, is the problem of dimer statistics [1]. The problem asks for a combinatorial solution to the number of ways of placing k dimers (dumbells) on a lattice containing N points, such that any two dimers are placed in a disjoint manner (i.e., two dimers do not have a common vertex in the lattice). This problem is considered an unsolved combinatorial problem [2], in general, for three-dimensional lattices. Even for two-dimensional and other lattices only special cases have been solved. The problem is not only mathematically intriguing but has many important applications in physics and chemistry. The grand canonical

* Dedicated to Professor V. Krishnamurthy on the occasion of his 60th birthday

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*** Alfred P. Sloan fellow; Camille and Henry Dreyfus teacher-scholar partition function of a lattice gas, the partition function of a system of interacting ferromagnets (the Ising problem), the kinetics and thermodynamics of adsorption of diatomics on surfaces, the enumeration of resonance chemical structures, and the stabilities of ionic crystals can all be shown to be related to dimer statistics [1–8].

While the complete dimer-covering problem (number of perfect matchings) has been solved for one-dimensional and two-dimensional lattices, a generating function for the number of ways of placing k dimers on a lattice of N points has not been solved to date, even for all two-dimensional lattices. The number of perfect matchings, however, can be obtained using the Pffafian expansion of the associated directed lattice [1] as reviewed in [1] or by the transfer matrix approach of Onsager [8]. An analytical solution for the complete covering of dimers has been obtained by Temperley and Fisher [9] and Kasteleyn [10] for square lattices.

A few mathematicians and graph theorists have obtained the generating functions for placing dimers on some graphs. They called these generating functions matching polynomials [11, 12]. Hosoya [13] was the first to define and use this generating function which he called the Z-counting polynomial. The matching polynomials of graphs and lattices are simply generating functions for the number of ways in placing disjoint dimers on lattices. The generating functions for the number of imperfect matchings (partial dimer coverings) have been obtained to date only for a few cases [14–16].

The matching polynomials and related polynomials of graphs of chemical interest have been obtained by many authors [16–29, 35, 36]. A computer code in Pascal has been developed to obtain matching polynomials of graphs [20]. Although there have been many such developments, applications to lattices lead to combinatorial explosions making these cases extremely challenging.

We show in the present investigation that analytical solutions for exact lattice statistics on linear, branched, cyclic and Bethe cacti lattices can easily be obtained by using a combination of the tree pruning method developed by one of the authors (K.B.) [27] and the operator methods [19]. Fisher and Essam [30] defined Bethe lattices and used them for percolation and cluster size problems. Subsequently, analytical expressions for some special cases of Bethe lattices [31] have been obtained. More recently the pruning methods have been developed for all Bethe isotropic and non-isotropic lattices [27].

A cactus lattice was defined by Uhlenbeck and Ford [32], and Husimi [33]. A cactus is a connected lattice in which no edge is shared by more than one cyclic subunit of the lattice. Farrell [34] very recently considered hexagonal cacti and obtained expressions for their matching polynomials. No general methods for deriving recursive relations and matching polynomials of cacti of any kind (branched, cyclic, crowned, etc.) containing rings of any size have been obtained to date. In this investigation, we combine the pruning method [27] with the operator technique [19] to derive general recursive relations for any cactus.

Section 2 outlines the pruning method and operator techniques for the characteristic polynomials and matching polynomials of cacti lattices. Section 3 comprises various applications of the operator and pruning methods. Sections

3.1 and 3.2 discuss the characteristic polynomials of cyclic and Bethe cacti, respectively. Sections 3.3, 3.4 and 3.5 consist of applications of the developed methods to matching polynomials of cacti, cyclic cacti lattices and Bethe cacti lattices. Section 3.6 describes the relationship between the characteristic and matching polynomials of cyclic cacti.

2. Pruning method and operator technique

2.1. Definitions and preliminaries

The adjacency matrix A of a graph is defined as a matrix in which an off-diagonal element is unity if the corresponding vertices are connected; otherwise it is zero. The secular determinant $|XI - A|$ where I is the $N \times N$ identity matrix (N = number of vertices) is called the characteristic polynomial. The matching polynomial, $M_G(x)$ of a graph is defined as

$$M_G(x) = \sum_{k=0}^{m} (-1)^k p(G, k) x^{N-2k}, \tag{1}$$

where $p(G, k)$ is the number of ways of placing k disjoint dimers in the graph G and m is the maximum number of dimers which can be placed on the lattice.

2.2. Pruning method

The pruning method was developed by one of the authors (K.B.) [27] for deriving characteristic or matching polynomials of trees. In this method, the given tree is pruned at various branch points successively until the final tree is simply a path. Then it was shown that the characteristic polynomial of the original tree can be synthesized in terms of the characteristic polynomials of the pruned tree and the fragments resulting in the process of pruning. Later this method was extended to graphs composed of cycles and branching ligands [37].

Figure 1 shows a simple square cactus containing five rings. The vertices at which two rings meet can be called the pruning points. The graphs should be pruned at these points successively. One of the authors (K.B.) [38] recently called

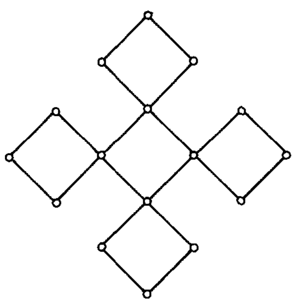

Fig. 1. A square cactus graph

such graphs spirographs and applied the pruning method to obtain characteristic polynomials, although no general analytical expression could be obtained for all graphs. In general, let S be called the core skeleton, and the branches (or ligands) be denoted by the set $\{L_i\}$. Then the parent graph G is given as the root-to-root product of S and the ligands, where root-to-root product was defined and illustrated in considerable detail by one of the authors (K.B.) in [41]. Symbolically, G can be expressed as $S \cup \{L_i\}$ where both S and the L_is need not be trees. The present method is applicable for any graph G as long as G can be expressed in the above form. The junction of L_i and S may be called the pivot point and denoted as p_i. Let M_i be defined as $L_i \ominus p_i$, where $\ominus$ means removal of the vertex p_i and all the edges incident to p_i (see Fig. 2) [18]. Let the characteristic polynomials of L_i and M_i be denoted as $\underline{L}_i$ and $\underline{M}_i$, respectively. If the adjacency matrix of S is denoted by A_{ij}, then the characteristic polynomial of the unpruned cactus, G, is the determinant of $\boldsymbol{H}$ given by

$$H_{ij} = \begin{cases} \underline{L}_i & \text{if } i = j \text{ and } i = p_i \\ x & \text{if } i = j \text{ and } i \neq p_i \\ -A_{ij}\underline{M}_i & \text{if } i \neq j \text{ and } i = p_i \\ -A_{ij} & \text{if } i \neq j \text{ and } i \neq p_i. \end{cases} \tag{2}$$

To illustrate the pruning method consider Fig. 2 (Fig. 1 is a special case of Fig. 2). Upon application of this method the characteristic polynomial of the cactus in Fig. 2 can be verified to be given by

$$P_G(x) = x^{16} - 20x^{14} + 144x^{12} - 464x^{10} + 640x^8 - 256x^6. \tag{3}$$

Although the above method can be used to generate the characteristic polynomials of various cacti and spirographs, it does not provide a closed analytical expression for the characteristic polynomials of cacti as a function of size. The operator technique described below achieves this.

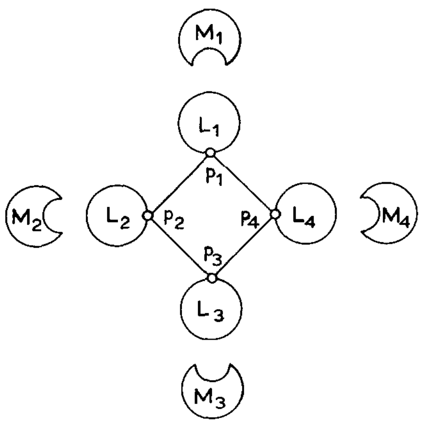

Fig. 2. The fragments L_1, L_2, L_3, L_4, M_1, M_2, M_3, M_4 obtained in pruning a general square cactus graph (see expression (7))

2.3. Operator technique

Hosoya and Ohkami [19] as well as Hosoya and Motoyama [16] have developed operator techniques for deriving recursive relations for characteristic and matching polynomials of graphs. We combine this technique with the pruning method to derive recursive expressions for various polynomials.

Let the set $\{C_i\}$ be a series of periodic graphs composed of a root C_0 with repetitive units (C_is) such that

$$C_n = C_{n+1} \ominus C \ (n \leqslant 0) \quad \text{or} \quad C_{n+1} = C_n \oplus C, \tag{4}$$

where $\oplus$ operation is the opposite of $\ominus$ operation defined before. Let $\hat{O}$ be a step-up operator for the characteristic polynomials of C_is. That is, $\hat{O}$ acts on C_n to yield C_{n+1}. To illustrate, consider a linear square cactus and the various C_is shown in Fig. 3.

Given a set of simultaneous recursive equations for the characteristic (or matching) polynomials for a family of graphs $\{A_n\}$, $\{B_n\}$, etc., which are derived from the same parent graph,

$$\begin{aligned}
&(a_{10}A_n + a_{11}A_{n-1} + \cdots + a_{1k}A_{n-k}) \\
&\quad + (b_{10}B_n + b_{11}B_{n-1} + \cdots + b_{1k}B_{n-k}) + \cdots = 0 \\
&(a_{20}A_n + a_{21}A_{n-1} + \cdots + a_{2k}A_{n-k}) \\
&\quad + (b_{20}B_n + b_{21}B_{n-1} + \cdots + b_{2k}B_{n-k}) + \cdots = 0
\end{aligned} \tag{5}$$

(the number of the series of graphs and the number of the independent recursive equations should be the same), then by the use of $\hat{O}$, the necessary condition for the existence of non-trivial solutions is as follows:

$$\begin{vmatrix}
a_{10}\hat{O}^k + a_{11}\hat{O}^{k-1} + \cdots + a_{1k} & b_{10}\hat{O}^k + b_{11}\hat{O}^{k-1} + \cdots + b_{1k} & \cdots \\
a_{20}\hat{O}^k + a_{21}\hat{O}^{k-1} + \cdots + a_{2k} & b_{20}\hat{O}^k + b_{21}\hat{O}^{k-1} + \cdots + b_{2k} & \cdots \\
 & \cdots &
\end{vmatrix} = 0 \tag{6}$$

The resultant operator polynomial, which is given by

$$C_0\hat{O}^l + C_1\hat{O}^{l-1} + C_2\hat{O}^{l-2} + \cdots + C_l = 0, \tag{7}$$

gives the recursive relation for the individual species of graphs $\{F_n\}$ ($F = A, B, \ldots$) as shown below:

$$C_0F_n + C_1F_{n-1} + \cdots + C_lF_{n-l} = 0. \tag{8}$$

Upon application of the operator technique to the pruning method for $P_G(x)$ of

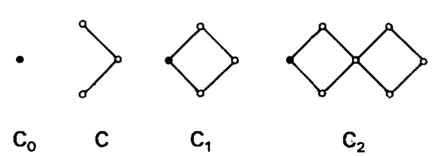

Fig. 3. The cacti graphs C_0, C, C_1, C_2, etc., in expression (9)

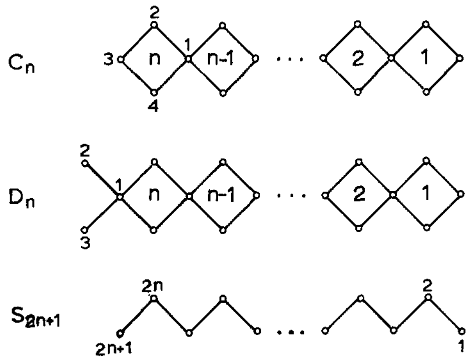

Fig. 4. The cacti which represent C_n, D_n and S_{n+1} for a linear square cactus

linear square cacti (see Fig. 4), one obtains

$$\begin{aligned} \{\underline{C}_n - (x^3 - 2x)\underline{C}_{n-1}\} + 2x^2\underline{D}_{n-2} \qquad &= 0 \\ -x^2\underline{C}_{n-1} \qquad + \{\underline{D}_{n-1} + 2x\underline{D}_{n-2}\} &= 0. \end{aligned}$$

The above expression can be expressed in terms of the operator $\hat{O}$ as

$$\begin{aligned} \{\hat{O}^2 - (x^3 - 2x)\hat{O}\}\underline{C}_{n-2} + 2x^2\underline{D}_{n-2} &= 0 \\ -x^2\hat{O}\underline{C}_{n-2} \quad + \{\hat{O} + 2x\}\underline{D}_{n-2} &= 0. \end{aligned} \tag{9}$$

In order for $\underline{C}_{n-2}$ and $\underline{D}_{n-2}$ to be non-trivial, the associated determinant of the coefficients should be zero. Consequently,

$$\hat{O}\{\hat{O}^2 - (x^3 - 4x)\hat{O} + 4x^2\} = 0. \tag{10}$$

This in turn yields

$$\underline{C}_n - (x^3 - 4x)\underline{C}_{n-1} + 4x^2\underline{C}_{n-2} = 0. \tag{11}$$

Note that this equation suggests one of the sufficient conditions. The following relation also holds for D_ns:

$$\underline{D}_n - (x^3 - 4x)\underline{D}_{n-1} + 4x^2\underline{D}_{n-2} = 0. \tag{12}$$

In Table 1, we give the results for other linear and kinked cacti.

We could obtain a general expression for the characteristic polynomial of linear cactus as shown below:

$$C_n(x) = \sum_{k=0}^{n}(-1)^k 2^k \binom{2n+1-k}{k} x^{3n+1-2k}. \tag{13}$$

The $C_n(x)$ can also be shown to be related to the Chebyshev polynomials for the path graph as follows (see also Fig. 4):

$$C_n(\sqrt{2}x) = 2^{\frac{3n+1}{2}} x^n S_{2n+1}(x), \tag{14}$$

where S_n is a Chebyshev polynomial, given by [39]

$$S_n(x) = \sum_{k=0}^{[n/2]}(-1)^k \binom{n-k}{k} x^{n-2k}. \tag{15}$$

Table 1. Recursive relations for the characteristic polynomials of linear and kinked cacti

Cactus type[a]	Characteristic polynomials
1	$C_n = (x^2 - 2)C_{n-1} - (x+1)^2 C_{n-2}$
2	$C_n = (x^3 - 4x)C_{n-1} - 4x^2 C_{n-2}$
3	$C_n = (x^3 - 3x)C_{n-1} - x^4 C_{n-2}$
4	$C_n = (x^4 - 5x^2 + 2)C_{n-1} - (x^2 + x - 1)^2 C_{n-2}$
5	$C_n = (x^4 - 4x^2 + 2)C_{n-1} - (x-1)^2(x^2 + x - 1)^2 C_{n-2}$
6	$C_n = x(x^2 - 1)(x^2 - 5)C_{n-1} - 4(x^2 - 1)C_{n-2}$
7	$C_n = (x^5 - 6x^3 + 6x)C_{n-1} - x^2(x^2 - 1)^2 C_{n-2}$
8	$C_n = (x^5 - 5x^3 + 5x)C_{n-1} - (x^2 - 1)^2(x^2 - 2)^2 C_{n-2}$

[a] See Fig. 5 for cactus types (1)–(8)

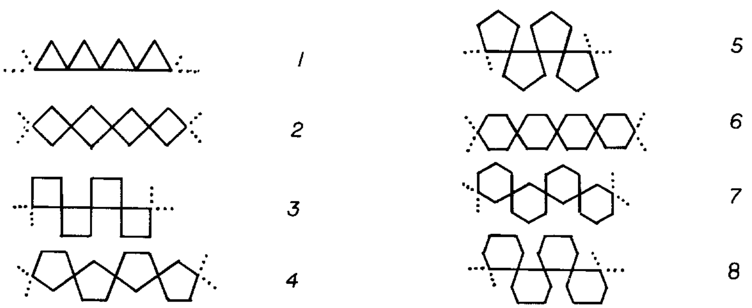

Fig. 5. Linear and kinked cacti containing cycles of varied sizes. For the characteristic and matching polynomials of these cacti see Tables 1 and 2, respectively

3. Applications

We consider in this section cyclic cacti of many kinds, Bethe cacti (branched) and other cacti.

3.1. *Characteristic polynomials of cyclic cacti*

There are two different types in cyclic cacti as in Fig. 6. Let us first consider the type in Fig. 6a with the fragments $\underline{L}$ and $\underline{M}$. If L and M denote the characteristic

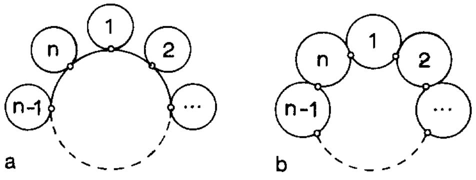

Fig. 6. Two types of cyclic cacti lattices

polynomials of these fragments, then the characteristic polynomial of the cactus in Fig. 6a is given as an $n \times n$ determinant shown below:

$$G_n = \underline{M}^n \begin{vmatrix} \underline{L}/\underline{M} & -1 & 0 & \cdots & -1 \\ -1 & \underline{L}/\underline{M} & -1 & \cdots & \\ 0 & -1 & \underline{L}/\underline{M} & \cdots & -1 \\ \cdot & & & \cdots & \underline{L}/\underline{M} \\ -1 & & & \cdots & -1 \end{vmatrix}$$

$$= \underline{M}^n \underline{C}_n(\underline{L}/\underline{M}) = M^n\{\underline{L}_n(\underline{L}/\underline{M}) - \underline{L}_{n-2}(\underline{L}/\underline{M}) - 2\}, \tag{16}$$

where $\underline{C}_n$ and $\underline{L}_n$ are the characteristic polynomials of cycle graph C_n and path graph L_n, respectively.

For the type in Fig. 6b, one can derive the recursive relations for the characteristic polynomials of cyclic cacti as follows. As explained in detail in [19], the recursive relation of the characteristic polynomial obtained by deleting an edge within a cycle carries extra terms to be added to the main terms corresponding to the matching polynomial. We need to find all the possible detour paths $\{\bar{l}_i\}$ connecting the two ends of the pivot edge l and subtract the contributions $2\sum_i G \ominus \bar{l}_i$.

Thus the characteristic polynomial R_n of the graph in Fig. 6b is decomposed into

$$\begin{aligned} R_n &= S_{n-1} - xE_{n-3} - 2E_{n-3} \\ &\quad -2x\left[x^{n-1} + (n-1)x^{n-2} + \binom{n-1}{2}x^{n-3} + \cdots + \binom{n-1}{n-1}\right] \\ &= S_{n-1} - (x+2)E_{n-3} - 2x(x+1)^{n-1}. \end{aligned} \tag{17}$$

The cyclic subgraph S_n can also be decomposed into

$$S_n = D_n - D_{n-1} - 2(x+1)^n. \tag{18}$$

This can in turn be simplified as

$$\begin{aligned} R_n - (x+1)R_{n-1} &= D_{n-1} - (x+2)D_{n-2} + (x+1)D_{n-3} \\ &\quad - (x+2)E_{n-3} + (x^2+2x+3)E_{n-4}. \end{aligned} \tag{19}$$

We can easily show by following the procedure explained for the linear square cacti that C_n, D_n and E_n obey the recursive relation,

$$f(\hat{O}, x)G_n = 0, \qquad G = C, D, E, \tag{20}$$

where

$$f(\hat{O}, x) = \hat{O}^2 - (x^2 - 2)\hat{O} + (x+1)^2 \quad \text{(see Table 1)}. \tag{21}$$

The left-hand side of Eq. (17) can be expressed as $\{\hat{O} - (x+1)\}R_{n-1}$, while each term in the right-hand side obeys Eq. (20). Thus one obtains

$$\begin{aligned}\{\hat{O}-(x+1)\}f(\hat{O},x)R_n &= \{\hat{O}-(x+1)\}\{\hat{O}^2-(x^2-2)\hat{O}+(x+1)^2\}\\ &= \hat{O}^3-(x^2+x-1)\hat{O}^2-(x^2+x-1)\\ &\quad\times(x+1)\hat{O}-(x+1)^3=0. \end{aligned}\tag{22}$$

Hence we have

$$R_n=(x^2+x-1)R_{n-1}-(x^2+x-1)(x+1)R_{n-2}+(x+1)^3R_{n-3}. \tag{23}$$

Similarly for the characteristic polynomial of cyclic tetragonal cacti we get

$$\begin{aligned}(\hat{O}-x^2)\{\hat{O}-(x^3-3x)\hat{O}+x^4\} &= \hat{O}^3-(x^3+x^2-3x)\hat{O}^2\\ &\quad+(x^5+x^4-3x^3)\hat{O}-x^6=0. \end{aligned}\tag{24}$$

3.2. Characteristic polynomials of Bethe cacti

The pruning-operator method could also be applied to Bethe cacti. Consider the Bethe cactus in Fig. 7 as an example. The recursive relation for the characteristic polynomials of a square Bethe cactus (see Fig. 7) is given by

$$\begin{aligned}&C_{n+1}=D_n^2(D_n^2-4E_n^2);\quad D_{n+1}=D_n\{x(D_n^2-2E_n^2)-2D_nE_n\};\\ &E_{n+1}=D_n(D_n^2-2E_n^2). \end{aligned}\tag{25}$$

For a triangular Bethe cactus (Fig. 8), the recursive relations are as follows:

$$\begin{aligned}&C_{n+1}=D_n^3-3E_n^2D_n-2E_n^3;\quad D_{n+1}=x(D_n^2-E_n^2)-2E_n(D_n+E_n);\\ &E_{n+1}=D_n^2-E_n^2. \end{aligned}\tag{26}$$

Similar recursive relations could be obtained for any Bethe cactus.

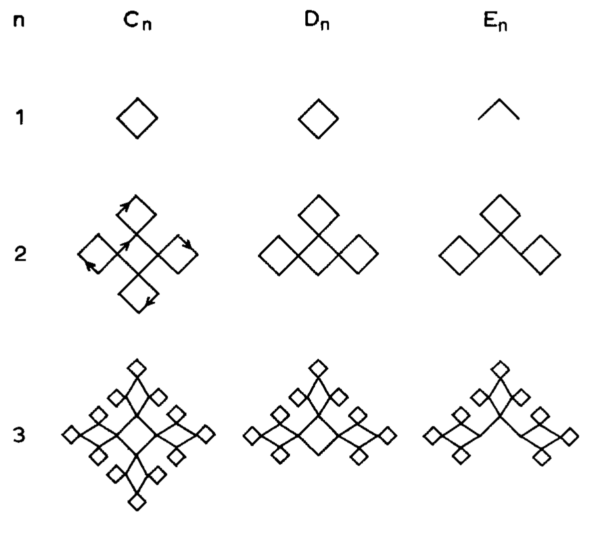

Fig. 7. Square Bethe cacti and subgraphs. C_2 represents the associated edge-weighted directed graph. *Arrows* in C_2 represent imaginary weights (see Sect. 3.3)

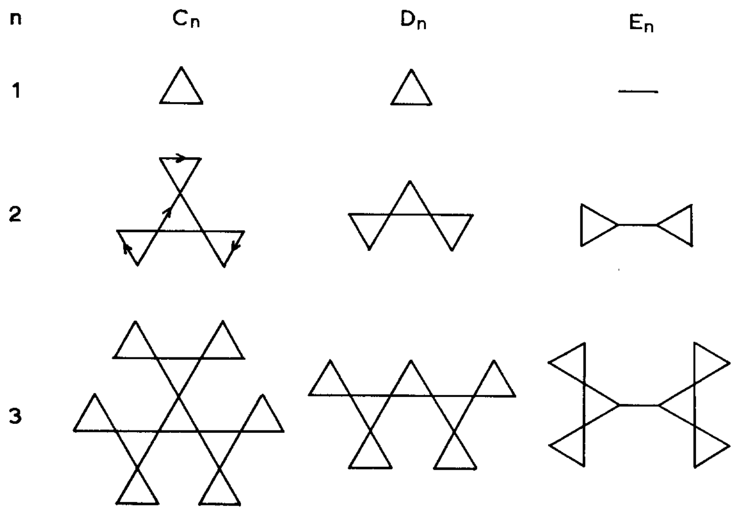

Fig. 8. Trigonal Bethe cacti and subgraphs. C_2 represents the associated edge-weighted directed graph. *Arrows* as for Fig. 7

3.3. Matching polynomials of cacti

Hosoya and Balasubramanian [29] have recently developed computational algorithms to obtain matching polynomials of graphs from the characteristic polynomials of associated edge-weighted directed graphs. In this section we show that when the pruning-operator method is applied to weighted cacti (some of the weights being imaginary numbers) one obtains the matching polynomials. To our knowledge, up to now no general technique such as this has been obtained for the matching polynomials of cacti.

Consider the linear square cactus shown in Fig. 4 as a starting example. An edge from each ring is chosen in the cactus and is weighted. This is shown in Fig. 9 with an arrow. The arrow indicates a weight of $+i$ in the direction of the arrow and a weight of $-i$ in the opposite direction so that the adjacency matrix of the resulting graph is Hermitian. We have shown before that the introduction of weights of $\pm i$ for each ring quenches its cyclic contribution [29]. Thus the characteristic polynomial of the resulting edge-weighted graph is the matching polynomial.

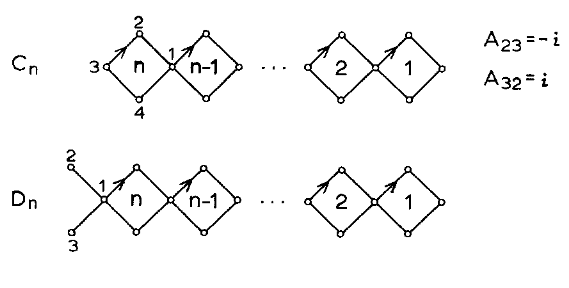

Fig. 9. Edge-weighted directed graph associated with a linear square cactus

The pruning-operator method can be applied to weighted and directed graphs as well. The application of this method for the linear square cactus yields the following relations:

$$\begin{aligned} \underline{C}_n &= (x^3 - 4x)\underline{C}_{n-1} - 2x^2\underline{C}_{n-2}, \\ \underline{D}_n &= (x^3 - 4x)\underline{D}_{n-1} - 2x^2\underline{D}_{n-2}. \end{aligned} \tag{27}$$

For convenience we express the above recursive relation in terms of an operator polynomial as

$$f(\hat{O}, x) = \hat{O}^2 - (x^3 - 4x)\hat{O} + 2x^2. \tag{28}$$

Note that the above method could be applied to any cactus. Similar recursive relations can be obtained for other linear cacti as well as kinked cacti. Table 2 shows recursive relations for many linear and kinked cacti lattices.

3.4. *Matching polynomials of cyclic cacti lattices*

The pruning-operator method can also be applied to cyclic cacti lattices containing cycles of any length. Consider the cyclic square cactus shown in Fig. 10 as an example. Let R_n be a cyclic square cactus and D_n, E_n be defined as shown in Fig. 10. $\underline{R}_n$, $\underline{D}_n$ and $\underline{E}_n$ are the characteristic polynomials of the corresponding

Table 2. Recursive relations for the matching polynomials of linear and cyclic cacti

Cactus type[a]	Matching polynomial
1	$C_n = (x^2 - 2)C_{n-1} - (x^2 + 1)C_{n-2}$
2	$C_n = (x^3 - 4x)C_{n-1} - 2x^2C_{n-2}$
3	$C_n = (x^3 - 3x)C_{n-1} - (x^4 - 2x^2 + 2)C_{n-2}$
4	$C_n = (x^4 - 5x^2 + 2)C_{n-1} - (x^4 - x^2 + 1)C_{n-2}$
5	$C_n = (x^4 - 4x^2 + 2)C_{n-1} - (x^6 - 4x^4 + 4x^2 + 1)C_{n-2}$
6	$C_n = x(x^2 - 1)(x^2 - 5)C_{n-1} - 2(x^2 - 1)^2C_{n-2}$
7	$C_n = (x^5 - 6x^3 + 6x)C_{n-1} - (x^6 - 4x^4 + 5x^2)C_{n-2}$
8	$C_n = (x^5 - 5x^3 + 5x)C_{n-1} - (x^8 - 6x^6 + 11x^4 - 6x^2 + 2)C_{n-2}$

[a] See Fig. 5 for cactus types (1)–(8)

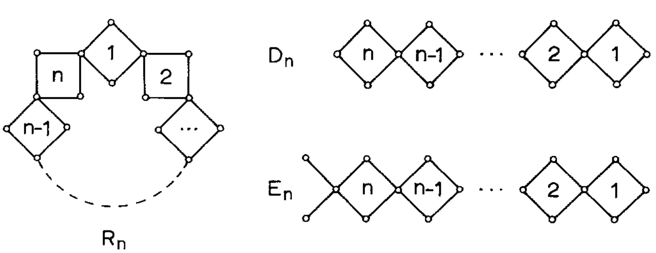

Fig. 10. The graphs R_n, D_n and E_n appearing in the recursive relation for cyclic cacti (see (30))

edge-weighted cacti. Then using the known recursive relation [13, 40] the matching polynomial of a cyclic spirograph can simply be expressed as

$$\underline{R}_n = 2\underline{D}_n - x\underline{E}_{n-2}, \tag{29}$$

where a point joining two squares was chosen as the pivot vertex. For D_n and E_n we use the characteristic polynomials of the associated edge-weighted graphs for deriving the relations among the matching polynomials. The final relation is given by

$$\begin{aligned} \underline{R}_n + x\underline{E}_{n-2} - 2\underline{D}_n &= 0, \\ \underline{E}_{n-1} + 2x\underline{E}_{n-2} - x^2\underline{D}_{n-1} &= 0, \\ f(\hat{O}, x)\underline{D}_n &= 0. \end{aligned} \tag{30}$$

It was found that this is also the case with the linear and cyclic cacti composed of polygons of any size, contrary to the observation by Farrell for hexagonal cacti [34]. These relationships were used to obtain the actual matching polynomials of many cacti up to octagonal cacti; numerical results can be obtained from the authors. This means that the operator polynomial for $\underline{R}_n$ might be $f(\hat{O}, x)$ or $(\hat{O} + 2x)f(\hat{O}, x)$. By using expressions for $\underline{R}_1$, $\underline{R}_2$ and $\underline{R}_3$ it was found that $f(\hat{O}, x)$ is also applicable to $\underline{R}_n$, namely,

$$\underline{R}_n = (x^3 - 4x)\underline{R}_{n-1} - 2x^2\underline{R}_{n-2}. \tag{31}$$

Consider as the next example the cacti in Fig. 11, where the mode of joining the squares is different from the case in Fig. 10. For these the pruning-operator method yields the following recursive relations:

$$\begin{aligned} &\underline{S}_n = 2\underline{T}_{n-1} - x\underline{U}_{n-2}, \\ &\underline{T}_n = (x^2 - 1)\underline{V}_n - x\underline{T}_{n-1}, \\ &\underline{U}_n = (x^2 - 1)\underline{T}_n - x\underline{U}_{n-1}, \\ &f(\hat{O}, x)\underline{V}_n = 0, \\ &f(\hat{O}, x) = \hat{O}^2 - (x^3 - 3x)\hat{O} + (x^2 - 2x^2 + 2). \end{aligned} \tag{32}$$

Also in this case, the $f(\hat{O}, x)$ is found to be applied to $\underline{S}_n$, together with $\underline{T}_n$ and $\underline{U}_n$.

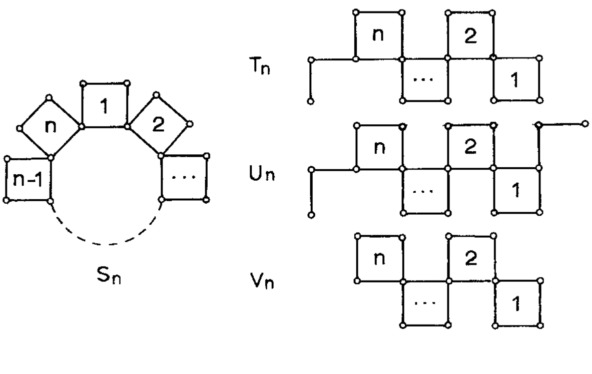

Fig. 11. The graphs S_n, T_n, U_n and V_n (see expression (32))

3.5. *Matching polynomials of Bethe cactus lattice*

A Bethe cactus lattice can be obtained by replacing each vertex of an ordinary Bethe lattice tree as defined by Fisher and Essam by a cyclic graph. An example of a Bethe cactus lattice is shown in Fig. 7. The matching polynomial of a Bethe cactus lattice can again be obtained using the pruning-operator method by weighting one edge of each cycle in the lattice by $\pm i$ such that the adjacency matrix of the weighted lattice is Hermitian. Figure 7 defines the various fragments C_n, D_n, E_n $(n = 1, 2, 3, \ldots)$ of a square Bethe lattice. Application of the pruning method to the associated edge-weighted directed graphs of Bethe lattice yields

$$C_{n+1} = (D_n^2 - 2E_n^2)^2 - 2E_n^4; \quad D_{n+1} = xD_n(D_n^2 - 2E_n^2) - 2E_n(D_n^2 - E_n^2);$$

$$E_{n+1} = D_n(D_n^2 - 2E_n^2). \tag{33}$$

It can easily be shown that the number of perfect matchings of C_n is given by

$$C_n(\text{const. coef}) = 2^{(3^n - 1)/2} \tag{34}$$

For the triangular Bethe cactus, define the various fragments with edge weights as in Fig. 12. Then one obtains the matching polynomial of the lattice as follows:

$$C_{n+1} = D_n(D_n^2 - 3E_n^2); \quad D_{n+1} = x(D_n^2 - E_n^2) - 2D_nE_n;$$

$$E_{n+1} = D_n^2 - E_n^2. \tag{35}$$

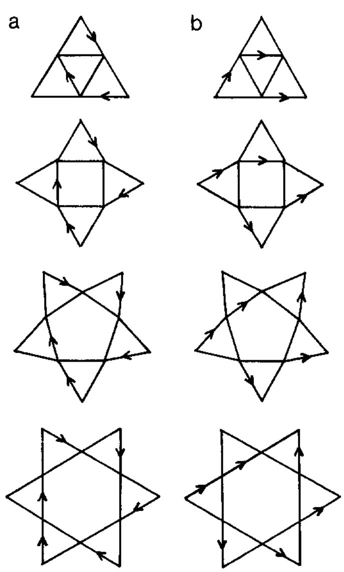

Fig. 12. Pairs of associated edge-weighted graphs whose characteristic polynomials give the matching polynomial

3.6. Relation between the characteristic polynomials and matching polynomials of cyclic cacti

We have already obtained the recursive relations of both the characteristic and matching polynomials of cyclic cacti in Sects. 3.1 and 3.4. In [29] we showed that contrary to the case of linear and kinked cacti, the matching polynomials of certain types of polycyclic graphs can be expressed as the mean of the characteristic polynomials of a set of edge-weighted directed graphs associated with the parent polycyclic graphs. As the numbers of vertices and cycles of graphs increase, the number of steps for obtaining the matching polynomials increases exponentially. Thus it is worth presenting the rigorous expressions of the $M_G(x)$ as linear combinations of the characteristic polynomials of edge-weighted directed graphs.

The results obtained for the cyclic triangular cacti are given in Fig. 12. These indicate that for each of the four cyclic triangular cacti $M_G(x)$ is obtained as the mean of the characteristic polynomials of the pair of associated edge-weighted directed graphs (Fig. 12a,b), where the arrow represents what has been explained in Sect. 3.3 and Fig. 9. In line with these pairs of graphs, one can continue to draw a pair of edge-weighted graphs for larger cyclic cacti of any size. One can also prove this algorithm inductively by following the procedure explained in [29]. Further, it is straightforward to show that the same method can be applied to other cyclic cacti composed of larger cycles.

References

1. Montroll E (1964) In: Beckenbach EF (ed) Applied combinatorial mathematics. Wiley, New York
2. Kasteleyn PW (1967) In: Harary F (ed) Graph theory and theoretical physics. Academic Press, London, p 43
3. Percus JK (1969) Combinatorial methods. Courant Institute of New York University, New York
4. Temperley HNV (1972) In: Domb C, Green MS (eds) Phase transitions and critical phenomena, vol 1. Academic Press, London, p 227
5. Harary F Graph theory. Addison-Wesley, Reading, Mass
6. Gordon M, Davison WHT (1952) J Chem Phys 20:428
7. Kilpatrick JE (1971) In: Rice S, Prigogine I (eds) Advances in chemical physics. Wiley, New York, p 1
8. Onsager L (1944) Phys Rev 65:117
9. Temperley HNV, Fisher ME (1961) Philos Mag 6:1061
10. Kasteleyn PW (1961) Physica 27:1209
11. Farrell EJ (1979) J Combinatorial Theory B 27:75
12. Gutman I (1979) Match 6;75
13. Hosoya H (1971) Bull Chem Soc Jpn 44:2332
14. McQuistan R B, Lichtman S J (1970) J Math Phys 11:3095
15. Hock HJ, McQuistan RB (1983) J Math Phys 24:1859
16. Hosoya H, Motoyama A (1985) J Math Phys 26:157
17. Hosoya H (1975) Theor Chim Acta 38:37
18. Hosoya H, Hosoi K (1976) J Chem Phys 64:1065
19. Hosoya H, Ohkami H (1983) J Comput Chem 4:585
20. Ramaraj R, Balasubramanian K (1985) J Comput Chem 6:122

21. Balasubramanian K (1986) In: Trinajstić N (ed) Mathematical and computational concepts in chemistry. Ellis Horwood, Chichester
22. Gutman I, Graovac A, Mohar B (1982) Match 13:129
23. Graovac A, Polansky OE (1986) Match 21:33
24. Polansky OE, Graovac A (1986) Match 21:46
25. Aihara J (1976) J Am Chem Soc 98:2570
26. Mohar B, Trinajstić N J (1982) Comput Chem 3:28
27. Balasubramanian K (1982) Int J Quantum Chem 21:581
28. Balasubramanian K (1988) J Math Chem 2:69
29. Hosoya H, Balasubramanian K (1989) J Comput Chem 16:698
30. Fisher ME, Essam JW (1961) J Math Phys 2:609
31. Heilmann OJ, Lieb EH (1972) Commun Math Phys 25:190
32. Uhlenbeck GE, Ford GW (1963) Lecture in statistical mechanics. Am Math Soc., Providence, RI
33. Husimi K (1975) J Chem Phys 18:682
34. Farrell EJ (1987) Int J Math Math Sci 10:321
35. Gutman I, Milan M, Trinajstić N (1975) Match 1:171; (1977) J Am Chem Soc 99:1692
36. Aihara J (1976) J Am Chem Soc 98:2750
37. Balasubramanian K, Randić M (1982) Theor Chim Acta 61:307
38. Balasubramanian K (in press) J Math Chem
39. Hosoya H, Randić M (1983) Theor Chim Acta 63:473
40. Hosoya H (1973) Fibonacci Quart 11:255
41. Balasubramanian K (1979) Theor Chim Acta 51:37