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HAFNIAN OF TWO-PARAMETER TOEPLITZ MATRICES

D.B. EFIMOV

ABSTRACT. Initially, the concept of **hafnian** appeared in the works on quantum field theory of the Italian theoretical physicist E.R. Caianiello. But **it also has** an important combinatorial property: the hafnian of the adjacency matrix of an undirected graph is equal to the number of perfect matchings **of** this graph. The use of hafnian is limited by complexity of its computation in **the** general case. In this paper we present an efficient method for exact **calculating** the hafnians of two-parameter Toeplitz matrices. This method is based on the formula expressing the hafnian of **the** sum of two matrices through the product of the hafnians of **matrices**. The necessary condition for **using** this method is also **the ability** to count the number of matchings **of** some arc diagrams. As an example, we propose a new interpretation of **some** sequences from On-Line Encyclopedia of Integer Sequences, give **a** new analytical formulas **to count** the number of some linear chord diagrams, and point out an interesting connection between the hafnian of two-parameter Toeplitz matrices and the Bessel polynomials.

Keywords: hafnian, arc diagram, perfect matching, Toeplitz matrix, chord diagram, Bessel polynomial.

1. INTRODUCTION

Let $A = (a_{ij})$ be a symmetric matrix of even order $2m$ over a commutative associative ring. Its hafnian is defined as

$$\text{Hf}(A) = \sum_{(i_1 i_2 | \dots | i_{2m-1} i_{2m})} a_{i_1 i_2} \dots a_{i_{2m-1} i_{2m}},$$

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where the sum runs over all partitions of the set $\{1, 2, \dots, 2m\}$ into disjoint pairs $(i_1 i_2), \dots, (i_{2m-1} i_{2m})$ up to the order of pairs and the order of elements in each pair. So, for example, if $m = 2$ then $\text{Hf}(A) = a_{12}a_{34} + a_{13}a_{24} + a_{14}a_{23}$. Equivalently, one can define the hafnian as

$$\text{Hf}(A) = \frac{1}{m!2^m} \sum_{\sigma \in S_{2m}} a_{\sigma(1), \sigma(2)} \cdots a_{\sigma(2m-1), \sigma(2m)},$$

where the sum runs over all permutations of the set $\{1, 2, \dots, 2m\}$. Note that diagonal elements of the matrix are not present in the definition of the hafnian. We will take them equal to zero for convenience. The hafnian was introduced by E. R. Caianiello in one of his works on quantum field theory [1]. He gave the name to the new matrix function in honor of Copenhagen (Lat. Hafnia), the place where the idea of this mathematical concept first occurred to him. By this name he also emphasized connection with Pfaffian introduced by A. Cayley in 19th century, from which the hafnian differs only by the signs of some components. Later it became clear that the hafnian also has a useful combinatorial property related to solving an important problem in graph theory: if M is the adjacency matrix of an unordered graph with even number of vertices, then $\text{Hf}(M)$ equals the total number of perfect matchings of the graph.

Unfortunately, the widespread use of the hafnian is limited by the complexity of its computation in the general case. Thus, in the recent work [2] of A. Björklund, B. Gupt and N. Quesada the currently fastest exact algorithm to compute the hafnian of an arbitrary complex $n \times n$ matrix is described. It runs in $O(n^3 2^{n/2})$ time, and, as the authors show, it seems to be close to optimal. But numerical benchmarks on the Titan supercomputer (the 7th place in the Top500 ranking as June 2018) indicated that it would require about a month and a half to compute the hafnian of a randomly generated 100×100 complex matrix using this algorithm.

Since in the general case calculation of the hafnian has a high computational complexity, the problem is actual of finding efficient analytical formulas expressing the hafnian for special classes of matrices. Thus, in many important cases (e.g., when considering adjacency matrices of planar graphs) one can reduce calculation of the hafnian of a given matrix to a much more efficient calculation of the Pfaffian for another matrix, associated with the former one by certain simple transformations (see [3, 4] and references therein).

Another special type of matrices arising in many applications is that of Toeplitz matrices. Recall that a matrix is called Toeplitz if all elements of every of its diagonals parallel to the main one are the same. It is obvious that a symmetric Toeplitz matrix is uniquely determined by its first row. Let $\lambda \subset \{2, \dots, 2m\}$, and let a, b be elements of some ring R . We denote by $T_{2m}(a, \lambda, b)$ a symmetric Toeplitz matrix of order $2m$ with zero main diagonal, whose elements in the first row and in the columns with numbers in λ are equal to a , and elements in the first row and in the columns with numbers in $\{2, \dots, 2m\} \setminus \lambda$ are equal to b . We call such Toeplitz matrices *two-parameter*. For example (dots denote zeros),

$$T_4(a, \{2, 4\}, b) = \begin{pmatrix} \cdot & a & b & a \\ a & \cdot & a & b \\ b & a & \cdot & a \\ a & b & a & \cdot \end{pmatrix}.$$

In our work we present an effective method for exact **computing** the hafnian of $T_{2m}(a, \lambda, b)$. This method is based on the formula expressing the hafnian of **the** sum of two matrices through the product of the hafnians of matrices, and is also closely linked with the combinatorial problem of counting the number of matchings of some arc diagrams. In connection with the problem under consideration we mention also **the** paper [5]. This work presents an efficient algorithm for exact **calculating** the hafnian of banded Toeplitz matrices. The sets of banded and two-parameter Toeplitz matrices intersect but not coincide.

The paper is organized as follows. In **section** 2 we consider some **necessary** definitions related to the notion of arc diagram. In section 3 we give **some** properties of the hafnian and present a general scheme for computing the hafnian of two-parameter Toeplitz matrices. In sections 4 and 5 we consider some special cases.

2. ARC DIAGRAMS

An arc diagram is a graph presentation method **where** all the vertices are located along a line in the plane, while all edges are drawn as arcs of circles (Fig. 1). The edges connecting adjacent vertices are also sometimes drawn as **segments** (arcs of the circle of infinite radius). We say that two vertices of an arc diagram are at a

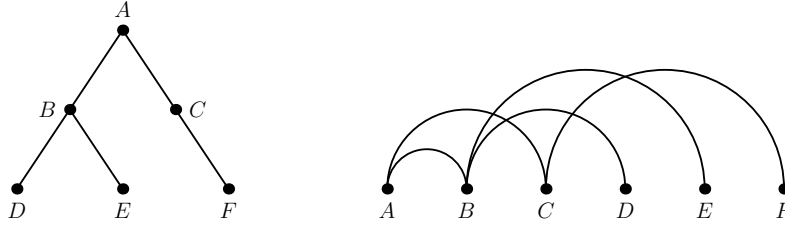


FIG. 1. A binary tree and its corresponding arc diagram

distance k from each other, if $k - 1$ vertices of the diagram are located between these vertices on the line. We also say that an arc connecting two such vertices is of length k . Thus, on the arc diagram shown in Fig. 1, the vertex C is connected to the vertex F by an arc of length 3.

Let $\lambda \subset \{1, 2, \dots, n - 1\}$. We say that an arc diagram with n vertices is λ -*complete* if it contains all possible arcs whose length value belongs to λ , and does not contain any other arcs. Thus, a $\{1\}$ -complete arc diagram is nothing else than a path graph (Fig. 2(a)). A $\{2\}$ -complete arc diagram is shown in Fig. 2(b).

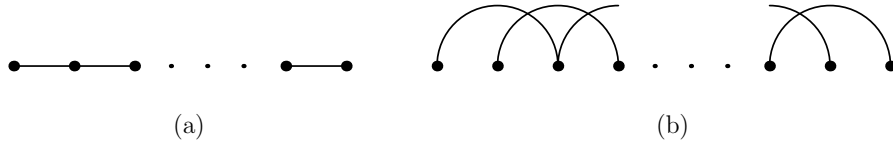


FIG. 2. (a) $\{1\}$ -complete arc diagram (a path graph); (b) $\{2\}$ -complete arc diagram

A *matching* **of** a graph is a set of pairwise non-adjacent edges. If a matching consists of k edges, then we say for convenience that **this** is a *k-edge matching*.

For example, all 2-edge matchings of $\{1\}$ - and $\{2\}$ -complete arc diagrams with 5 vertices are represented on Fig. 3. A *perfect matching* in a graph with $2m$ vertices is

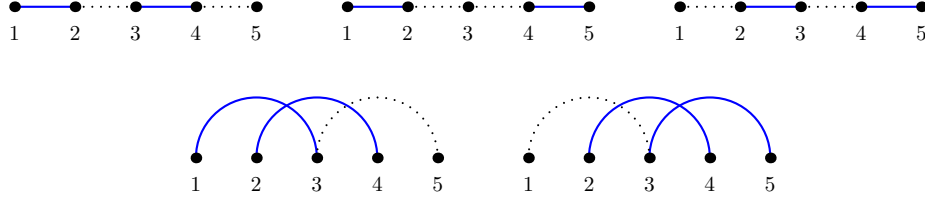


FIG. 3. The 2-edge matchings of $\{1\}$ - and $\{2\}$ -complete arc diagrams with 5 vertices

a matching consisting of m edges. Perfect matchings of arc diagrams are also called *linear chord diagrams* [6, 7].

Given a λ -complete arc diagram with n vertices, let $M_{n,k}(\lambda)$ denote the number of all its k -edge matchings. By definition we set $M_{n,0}(\lambda) = 1$.

Let a, b be nonnegative integers, and $\lambda \subset \{1, 2, \dots, 2m-1\}$. We denote by $G_{2m}(a, \lambda, b)$ an arc diagram with $2m$ vertices having the following form: if the distance between its two vertices belongs to λ then these vertices are connected by a arcs, otherwise by b arcs (Fig. 4).

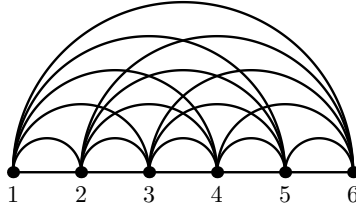


FIG. 4. The arc diagram $G_6(2, \{1\}, 1)$

Now let $\lambda \subset \{2, 3, \dots, 2m\}$. We denote by $\tilde{\lambda}$ a subset of $\{1, \dots, 2m-1\}$ which is obtained from λ by subtracting 1 from each of its elements: $\lambda = \{n_1, n_2, \dots, n_k\} \Rightarrow \tilde{\lambda} = \{n_1-1, n_2-1, \dots, n_k-1\}$. It is not hard to see that the two-parameter Toeplitz matrix $T_{2m}(a, \lambda, b)$ is the adjacency matrix of the arc diagram $G_{2m}(a, \tilde{\lambda}, b)$, and therefore the hafnian $\text{Hf}(T_{2m}(a, \lambda, b))$ represents the number of perfect matchings of $G_{2m}(a, \tilde{\lambda}, b)$.

3. HAFNIAN OF TWO-PARAMETER TOEPLITZ MATRICES

To begin with, consider two properties of the hafnian. The first property is quite obvious.

Proposition 1. *Let A be a symmetric matrix of order $2m$ over a commutative associative ring R , and $c \in R$. Then*

$$(1) \quad \text{Hf}(cA) = c^m \text{Hf}(A).$$

Let $Q_{k,n}$ denote the set of all unordered k -element subsets of the set $\{1, 2, \dots, n\}$. Let A be a matrix of order n and $\alpha \in Q_{k,n}$. We denote by $A[\alpha]$ the submatrix of A formed by the rows and columns of A with numbers in α , and by $A\{\alpha\}$ the submatrix of A formed from A by removing the rows and columns with numbers in α . The following property proved in [8]:

Proposition 2. *Let A, B be symmetric matrices of order $2m$. Then*

$$(2) \quad \text{Hf}(A + B) = \sum_{k=0}^m \sum_{\alpha \in Q_{2k, 2m}} \text{Hf}(A[\alpha]) \text{Hf}(B\{\alpha\}),$$

where $\text{Hf}(A[\alpha]) = 1$ if $\alpha \in Q_{0, 2m}$, and $\text{Hf}(B\{\alpha\}) = 1$ if $\alpha \in Q_{2m, 2m}$.

Let $\lambda \subset \{2, \dots, 2m\}$. We denote by $D_{2m}(q, \lambda)$ a symmetric Toeplitz matrix of order $2m$ whose elements in the first row and in columns with numbers from λ are equal to q and all other elements are equal to 0. We denote by $J_{2m}(q)$ a symmetric Toeplitz matrix of order $2m$ whose elements outside the main diagonal are equal to q . For example,

$$D_4(q, \{2, 4\}) = \begin{pmatrix} \cdot & q & \cdot & q \\ q & \cdot & q & \cdot \\ \cdot & q & \cdot & q \\ q & \cdot & q & \cdot \end{pmatrix}, \quad J_4(q) = \begin{pmatrix} \cdot & q & q & q \\ q & \cdot & q & q \\ q & q & \cdot & q \\ q & q & q & \cdot \end{pmatrix}.$$

Directly from a definition of the hafnian it follows that

$$(3) \quad \text{Hf}(J_{2m}(q)) = q^m \frac{(2m)!}{m!2^m}.$$

Since $T_{2m}(a, \lambda, b) = J_{2m}(b) + D_{2m}(a - b, \lambda)$, using the formulas (1), (2), and (3), we can write the following chain of equalities:

$$(4) \quad \begin{aligned} \text{Hf}(T_{2m}(a, \lambda, b)) &= \text{Hf}(J_{2m}(b) + D_{2m}(a - b, \lambda)) = \\ &= \sum_{k=0}^m \sum_{\alpha \in Q_{2k, 2m}} \text{Hf}(J_{2m}(b)[\alpha]) \text{Hf}(D_{2m}(a - b, \lambda)\{\alpha\}) = \\ &= \sum_{k=0}^m (a - b)^{m-k} b^k \frac{(2k)!}{k!2^k} \sum_{\alpha \in Q_{2k, 2m}} \text{Hf}(D_{2m}(1, \lambda)\{\alpha\}). \end{aligned}$$

Here we use the fact that the matrix $J_{2m}(b)[\alpha]$ has the same form as the initial matrix $J_{2m}(b)$, i.e., $J_{2m}(b)[\alpha]$ is a symmetric matrix of order $2k$ whose elements on the main diagonal are zero, and all others elements equal b .

Let d_{ij} denote the elements of the matrix $D_{2m}(1, \lambda)$. It is easy to see that elements of the form $d_{i, i+r}$ and $d_{i+r, i}$, where $r \in \tilde{\lambda}$, are equal to 1, and all others elements d_{ij} are equal to 0. If $\alpha \in Q_{2k, 2m}$, then the matrix $D_{2m}(1, \lambda)\{\alpha\}$ has the order $2m - 2k$, and, by definition,

$$(5) \quad \sum_{\alpha \in Q_{2k, 2m}} \text{Hf}(D_{2m}(1, \lambda)\{\alpha\}) = \sum_{\alpha \in Q_{2k, 2m}} \sum_P d_{i_1 j_1} \dots d_{i_{m-k} j_{m-k}},$$

where the inner sum runs over all partitions P of the set $\{1, 2, \dots, 2m\} \setminus \alpha$ into disjoint pairs $(i_1 j_1), \dots, (i_{m-k} j_{m-k})$ up to an order of pairs and an order of elements in each pair. It follows from the above that the term $d_{i_1 j_1} \dots d_{i_{m-k} j_{m-k}}$ in the sum (5) equals 1 if and only if the values $|i_1 - j_1|, \dots, |i_{m-k} - j_{m-k}|$ belong to $\tilde{\lambda}$. Otherwise the term $d_{i_1 j_1} \dots d_{i_{m-k} j_{m-k}}$ equals zero. It follows that the sum (5)

equals the number of different ways of choosing in $\{1, 2, \dots, 2m\}$ a set of $m - k$ disjoint pairs $(i_1, i_1 + r_1), \dots, (i_{m-k}, i_{m-k} + r_{m-k})$ where $r_1, \dots, r_{m-k} \in \tilde{\lambda}$ up to an order of pairs. And this is nothing but the number of $(m - k)$ -edge matchings of the $\tilde{\lambda}$ -complete arc diagram with $2m$ vertices, i.e., the number $M_{2m, m-k}(\tilde{\lambda})$. Substituting this value in (4), we get the expression:

$$(6) \quad \text{Hf}(T_{2m}(a, \lambda, b)) = \sum_{k=0}^m (a - b)^{m-k} b^k \frac{(2k)!}{k! 2^k} M_{2m, m-k}(\tilde{\lambda}).$$

Thus to calculate the hafnian of a two-parameter Toeplitz matrix by formula (6) one needs to determine the number of k -edge matchings of λ -complete arc diagrams. In general, this is non-trivial task. In the following sections we consider some special cases.

4. THE HAFNIAN OF $T_{2m}(a, \{2\}, b)$

Proposition 3. *Let k, n be nonnegative integers such that $k \leq \lfloor \frac{n}{2} \rfloor$. Then the number of k -edge matchings of $\{1\}$ -complete arc diagram with n vertices is equal to the binomial coefficient C_{n-k}^k :*

$$M_{n,k}(\{1\}) = C_{n-k}^k.$$

Proof. This statement can be proved in various ways. We apply the method of generating functions. For convenience, we shall use the notation $u_{n,k}$ rather than $M_{n,k}(\{1\})$ for the number of k -edge matchings in a $\{1\}$ -complete arc diagram with n vertices. It is easy to see that $u_{n,k}$ satisfy the recurrence relation

$$(7) \quad u_{n+2,k+1} = u_{n+1,k+1} + u_{n,k}$$

with the initial conditions: $u_{n,k} = 0$ for $k > \lfloor \frac{n}{2} \rfloor$, $u_{n,0} = 1$ for all n . Indeed, one can split the set of all k -edge matchings of a $\{1\}$ -complete arc diagram into the set of matchings containing the edge incident to the first left vertex, and the set of matchings that do not contain an edge incident to this vertex. To find the solution of the relation (7) in explicit form consider the generating function $u(x, t)$ for the sequence $u_{n,k}$:

$$u(x, t) = \sum_{n=0}^{+\infty} \sum_{k=0}^{+\infty} u_{n,k} x^k t^n = \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} u_{n,k} x^k t^n.$$

Multiplying (7) by $x^{k+1} t^{n+1}$ and summing over all possible k and n yields the following equation:

$$(8) \quad \begin{aligned} & \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} u_{n+2,k+1} x^{k+1} t^{n+1} = \\ & = \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} u_{n+1,k+1} x^{k+1} t^{n+1} + \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} u_{n,k} x^{k+1} t^{n+1}. \end{aligned}$$

Consider separately the formal power series ~~included in it~~. We have

$$\begin{aligned} \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} u_{n+1,k+1} x^{k+1} t^{n+1} &= u(x, t) - (u_{0,0} + u_{1,0}t + u_{2,0}t^2 + \dots) = \\ &= u(x, t) - \sum_{n=0}^{+\infty} t^n = u(x, t) - \frac{1}{1-t}. \end{aligned}$$

In a similar way,

$$\begin{aligned} \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} u_{n+2,k+1} x^{k+1} t^{n+1} &= \frac{1}{t} \left(\sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} u_{n+2,k+1} x^{k+1} t^{n+2} \right) = \\ &= \frac{1}{t} \left(u(x, t) - \sum_{n=0}^{+\infty} t^n \right) = \frac{1}{t} \left(u(x, t) - \frac{1}{1-t} \right). \end{aligned}$$

Finally, we obtain:

$$\sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} u_{n,k} x^{k+1} t^{n+1} = xtu(x, t).$$

Substituting these expressions to (8), we get

$$\frac{1}{t} \left(u(x, t) - \frac{1}{1-t} \right) = u(x, t) - \frac{1}{1-t} + xtu(x, t).$$

Solving this equation, we find the expression for $u(x, t)$ in the form of a formal power series:

$$(9) \quad u(x, t) = \frac{1}{1 - (t + xt^2)} = \sum_{m=0}^{+\infty} (t + xt^2)^m = \sum_{m=0}^{+\infty} \sum_{k=0}^m C_m^k x^k t^{m+k}.$$

Let $n = m + k$. Then the coefficient for $x^k t^n$ in (9), i.e. $u_{n,k}$, equals C_{n-k}^k . $\square$

Let R be a commutative associative ring with 1 and $a, b \in R$. Consider a symmetric two-parameter Toeplitz matrix $T_{2m}(a, \{2\}, b)$. Its order is $2m$ and its first row has the form:

$$(0 \quad a \quad b \quad \dots \quad b).$$

Theorem 1. *If we assume that $0^0 = 1$, then the hafnian of the matrix $T_{2m}(a, \{2\}, b)$ one can calculate using the following formula:*

$$(10) \quad \text{Hf}(T_{2m}(a, \{2\}, b)) = \sum_{k=0}^m (a-b)^{m-k} b^k \frac{(m+k)!}{k!(m-k)!2^k}.$$

Proof. By Proposition 3 $M_{2m,m-k}(\{1\}) = C_{m+k}^{m-k}$. Then substituting $\lambda = \{2\}$ in (6), we get the required equality:

$$\begin{aligned} \text{Hf}(T_{2m}(a, \{2\}, b)) &= \sum_{k=0}^m (a-b)^{m-k} b^k \frac{(2k)!}{k!2^k} M_{2m,m-k}(\{1\}) = \\ &= \sum_{k=0}^m (a-b)^{m-k} b^k \frac{(2k)!}{k!2^k} C_{m+k}^{m-k} = \sum_{k=0}^m (a-b)^{m-k} b^k \frac{(m+k)!}{k!(m-k)!2^k}. \end{aligned}$$

$\square$

Remark 1. Based on the formula (10), it is not hard to write an algorithm which calculates the hafnian of the matrix $T_{2m}(a, \{2\}, b)$ of order $2m$ in time $O(m)$.

Example 1. Consider the matrix $T_{2m}(0, \{2\}, 1)$. Its adjacency matrix is the arc diagram $G_{2m}(0, \{1\}, 1)$ (the complement of the path graph P_{2m}) (Fig. 5). It is not hard to see that perfect matchings of $G_{2m}(0, \{1\}, 1)$ are loopless linear chord diagrams with m chords considered in [6]. From (10) we get

$$(11) \quad \text{Hf}(T_{2m}(0, \{2\}, 1)) = \sum_{k=0}^m (-1)^{m-k} \frac{(m+k)!}{k!(m-k)!2^k}.$$

Thus, the formula (11) expresses the number of loopless linear chord diagrams with m chords (the sequence A278990 in [9]).

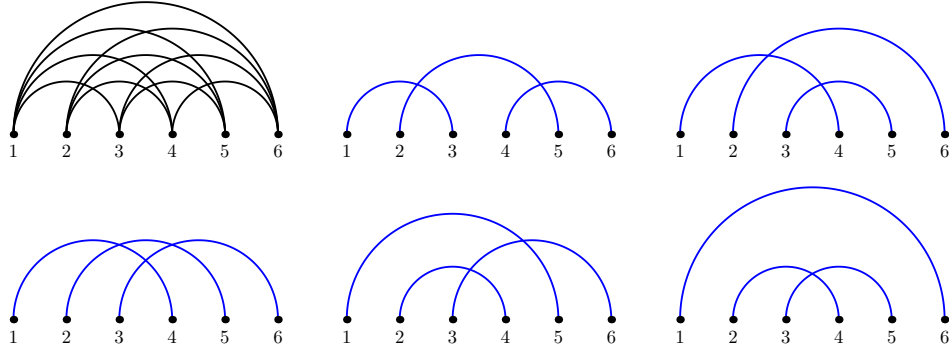


FIG. 5. The arc diagram $G_6(0, \{1\}, 1)$ and all its perfect matchings

Example 2. Consider the matrix $T_{2m}(2, \{2\}, 1)$. If one calculates by (10) its hafnian for consecutive m , then we get the sequence:

m	1	2	3	4	5	6	7	8	9	...
Hf	2	7	37	266	2431	27007	353522	5329837	90960751	...

It follows from the above that its m -th member equals the number of perfect matchings of the arc diagram $G_{2m}(2, \{1\}, 1)$ (Fig. 6). Note that this sequence has

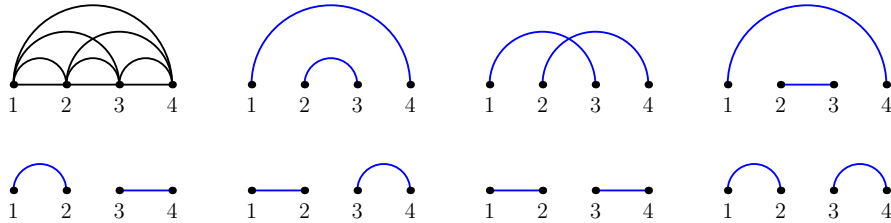


FIG. 6. The arc diagram $G_4(2, \{1\}, 1)$ and all its perfect matchings

the number A001515 in [9], but its description does not contain the interpretation given here.

Example 3. Recall (see [10], [11]) that the *Bessel polynomial* of degree m is a polynomial of the form:

$$y_m(x) = \sum_{k=0}^m \frac{(m+k)!}{k!(m-k)!} \left(\frac{x}{2}\right)^k.$$

It follows from (10) that the hafnian of the matrix $T_{2m}(b+1, \{2\}, b)$ equals the value of the Bessel polynomial of degree m at $x = b$:

$$\text{Hf}(T_{2m}(b+1, \{2\}, b)) = y_m(b).$$

This is a rather curious and unexpected fact, the explanation of which is not yet completely clear.

5. HAFNIAN OF MATRICES $T_{2m}(a, \{3\}, b)$

Proposition 4. Let k, n be a pair of nonnegative integers. Suppose that $n \neq 2k$ when k is odd. Then the inequality

$$(12) \quad \left\lceil \frac{3k-n}{2} \right\rceil \leq \left\lfloor \frac{k}{2} \right\rfloor$$

is equivalent to

$$(13) \quad k \leq \left\lfloor \frac{n}{2} \right\rfloor.$$

Proof. Suppose that (13) is wrong. This means that $n = 2k - c$, where $c \geq 1$. Substituting this value to the inequality (12), we see that it is wrong as well. Suppose now that (13) is true. Then $n = 2k + c$ and $\left\lceil \frac{3k-n}{2} \right\rceil = \left\lceil \frac{k-c}{2} \right\rceil$, where $c \geq 0$. If k is even, then $\left\lceil \frac{k-c}{2} \right\rceil$ does not exceed $\left\lfloor \frac{k}{2} \right\rfloor$. If k is odd, then, by the assumption, $n \neq 2k$. Therefore $c > 0$ and $\left\lceil \frac{k-c}{2} \right\rceil$ also does not exceed $\left\lfloor \frac{k}{2} \right\rfloor$. Thus, the inequality (12) also holds. $\square$

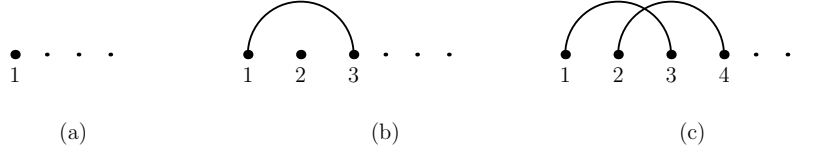
Proposition 5. Let k, n be a pair of non-negative integers. If $k \leq \left\lfloor \frac{n}{2} \right\rfloor$, but $n \neq 2k$ when k is odd, then the number of k -edged matchings of $\{2\}$ -complete arc diagram with n vertices is equal to the following sum:

$$(14) \quad M_{n,k}(\{2\}) = \sum_{i=\max(0, \left\lceil \frac{3k-n}{2} \right\rceil)}^{\left\lfloor \frac{k}{2} \right\rfloor} C_{n-2k+i}^{k-i} C_{k-i}^i.$$

Otherwise $M_{n,k}(\{2\}) = 0$.

Proof. For convenience, we shall use the abbreviated notation $v_{n,k}$ for $M_{n,k}(\{2\})$. Consider a k -edged matching of $\{2\}$ -complete arc diagram with n vertices. It is obvious that if $k > \left\lfloor \frac{n}{2} \right\rfloor$ then $v_{n,k} = 0$. If $n \geq 4$ then the following three cases are possible: the first vertex of the diagram is not incident to an edge of the matching (Fig. 7(a)); the first vertex is incident to an edge of the matching, but the second one is not (Fig. 7(b)); the first and the second vertices are incident to edges of the matching (Fig. 7(c)). It follows from the above that $v_{n,k}$ satisfy the recurrence relation

$$(15) \quad v_{n+4,k+2} = v_{n+3,k+2} + v_{n+1,k+1} + v_{n,k}$$

FIG. 7. Possible cases of matchings of $\{2\}$ -complete arc diagram

with the initial conditions: $v_{n,k} = 0$ for $k > \lfloor \frac{n}{2} \rfloor$; $v_{2,1} = 0$; $v_{n,0} = 1$ for all n ; $v_{n,1} = n - 2$ for $n \geq 2$. Consider the two-parameter generating function $v(x, t)$ for the sequence $v_{n,k}$:

$$v(x, t) = \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n,k} x^k t^n.$$

Multiplying (15) by $x^{k+3}t^{n+3}$ and summing over all possible k and n gives the following equation:

$$(16) \quad \begin{aligned} \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n+4,k+2} x^{k+3} t^{n+3} &= \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n+3,k+2} x^{k+3} t^{n+3} + \\ &+ \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n+1,k+1} x^{k+3} t^{n+3} + \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n,k} x^{k+3} t^{n+3}. \end{aligned}$$

Consider separately the formal power series on the left side of this equation.

$$\begin{aligned} \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n+4,k+2} x^{k+3} t^{n+3} &= \frac{x}{t} \left(\sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n+4,k+2} x^{k+2} t^{n+4} \right) = \\ &= \frac{x}{t} \left(v(x, t) - \sum_{n=0}^{+\infty} v_{n,0} t^n - \sum_{n=1}^{+\infty} v_{n,1} x t^n \right) = \\ &= \frac{x}{t} \left(v(x, t) - \sum_{n=0}^{+\infty} t^n - x \sum_{n=3}^{+\infty} (n-2) t^n \right) = \\ &= \frac{x}{t} \left(v(x, t) - \frac{1}{1-t} - x t^3 \left(\sum_{n=1}^{+\infty} t^n \right)' \right) = \\ &= \frac{x}{t} \left(v(x, t) - \frac{1}{1-t} - \frac{x t^3}{(1-t)^2} \right). \end{aligned}$$

In the same way, we get

$$\sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n+3,k+2} x^{k+3} t^{n+3} = x \left(v(x, t) - \frac{1}{1-t} - \frac{x t^3}{(1-t)^2} \right).$$

Also,

$$\begin{aligned} \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n+1,k+1} x^{k+3} t^{n+3} &= x^2 t^2 \sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n+1,k+1} x^{k+1} t^{n+1} = \\ &= x^2 t^2 \left(v(x, t) - \sum_{n=0}^{+\infty} v_{n,0} t^n \right) = x^2 t^2 \left(v(x, t) - \frac{1}{1-t} \right). \end{aligned}$$

Finally,

$$\sum_{n=0}^{+\infty} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} v_{n,k} x^{k+3} t^{n+3} = x^3 t^3 v(x, t).$$

Substituting all this to (16), we get

$$\begin{aligned} \frac{x}{t} \left(v(x, t) - \frac{1}{1-t} - \frac{xt^3}{(1-t)^2} \right) &= x \left(v(x, t) - \frac{1}{1-t} - \frac{xt^3}{(1-t)^2} \right) + \\ &+ x^2 t^2 \left(v(x, t) - \frac{1}{1-t} \right) + x^3 t^3 v(x, t). \end{aligned}$$

Solving this equation, we obtain:

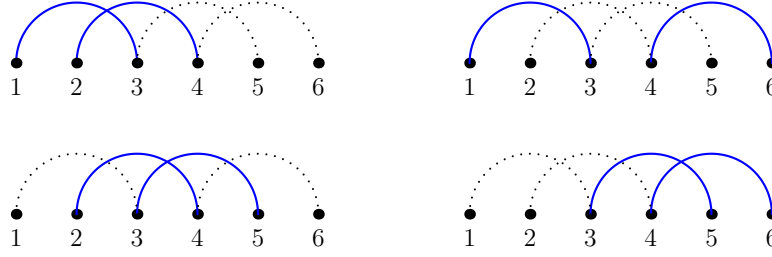
$$\begin{aligned} (17) \quad v(x, t) &= \frac{1}{1-t(1+xt^2+x^2t^3)} = \sum_{m=0}^{+\infty} t^m (1+xt^2+x^2t^3)^m = \\ &= \sum_{m=0}^{+\infty} t^m \sum_{j=0}^m C_m^j (xt^2+x^2t^3)^j = \sum_{m=0}^{+\infty} \sum_{j=0}^m C_m^j x^j t^{m+2j} (1+xt)^j = \\ &= \sum_{m=0}^{+\infty} \sum_{j=0}^m C_m^j x^j t^{m+2j} \sum_{i=0}^j C_j^i (xt)^i = \sum_{m=0}^{+\infty} \sum_{j=0}^m \sum_{i=0}^j C_m^j C_j^i x^{j+i} t^{m+2j+i}. \end{aligned}$$

Fix nonnegative integers k, n . From (17) we see that the coefficient at $x^k t^n$ is equal to $\sum_i C_{n-2k+i}^{k-i} C_{k-i}^i$ over all i for which the inequalities $i \geq 0$, $k-i \geq i$, $n-2k+i \geq k-i$ hold. The last two inequalities can be rewritten as $i \leq \lfloor \frac{k}{2} \rfloor$, $i \geq \lceil \frac{3k-n}{2} \rceil$. Thus, in order for the set of acceptable values of i to be non-empty, it is necessary that $\lceil \frac{3k-n}{2} \rceil \leq \lfloor \frac{k}{2} \rfloor$. But by Proposition 4, this condition is equivalent to $k \leq \lfloor \frac{n}{2} \rfloor$ except for the case when k is odd and $n = 2k$. In the last case, one immediately sees that the inequality $\lceil \frac{3k-n}{2} \rceil \leq \lfloor \frac{k}{2} \rfloor$ does not hold, and therefore the coefficient at $x^k t^n$ is equal to zero. This completes the proof. $\square$

Example 4. Here we calculate the number of 2-edge matchings of $\{2\}$ -complete arc diagram with 6 vertices. We have, therefore $n = 6$, $k = 2$, $\lfloor \frac{k}{2} \rfloor = 1$, $\lceil \frac{3k-n}{2} \rceil = 0$. Using (14), we get:

$$M_{6,2}(\{2\}) = \sum_{i=0}^1 C_{2+i}^{2-i} C_{2-i}^i = C_2^2 C_2^0 + C_3^1 C_1^1 = 1 \cdot 1 + 3 \cdot 1 = 4.$$

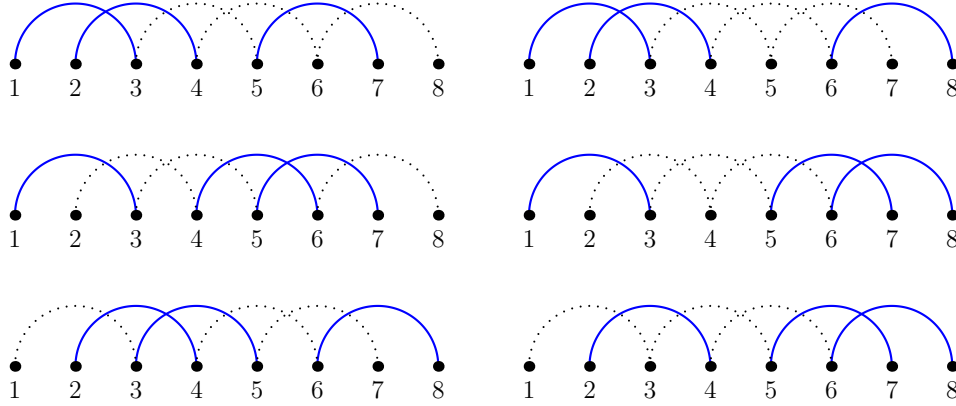
All these matchings are shown on Fig. 8.

FIG. 8. All 2-edge matchings of $\{2\}$ -complete arc diagram with 6 vertices

Example 5. Now we calculate the number of 3-edge matchings of $\{2\}$ -complete arc diagram with 8 vertices. We have $n = 8$, $k = 3$, $\lfloor \frac{k}{2} \rfloor = 1$, $\lceil \frac{3k-n}{2} \rceil = 1$. Using (14), we obtain:

$$M_{8,3}(\{2\}) = \sum_{i=1}^1 C_{2+i}^{3-i} C_{3-i}^i = C_3^2 C_2^1 = 3 \cdot 2 = 6.$$

All these matchings are shown on Fig. 9.

FIG. 9. All 3-edge matchings of $\{2\}$ -complete arc diagram with 8 vertices

Let R be a commutative associative ring with 1, and let $a, b \in R$. Consider a symmetric two-parameter Toeplitz matrix $T_{2m}(a, \{3\}, b)$. Its order is $2m$, and its first row has the form:

$$(0 \quad b \quad a \quad b \quad \dots \quad b).$$

Theorem 2. If we assume that $0^0 = 1$, then the hafnian of the matrix $T_{2m}(a, \{3\}, b)$ can be calculated using the following formula:

$$(18) \quad \begin{aligned} \text{Hf}(T_{2m}(a, \{3\}, b)) &= \\ &= \sum_{k=p}^m (a-b)^{m-k} b^k \frac{(2k)!}{k! 2^k} \sum_{i=\max(0, \lceil \frac{m-3k}{2} \rceil)}^{\lfloor \frac{m-k}{2} \rfloor} C_{2k+i}^{m-k-i} \cdot C_{m-k-i}^i, \end{aligned}$$

where $p = 0$ when m is even, and $p = 1$ when m is odd.

Proof. By Proposition 5 we have two cases. If $2m = 2(m - k)$ and $m - k$ is odd, or equivalently, if $k = 0$ and m is odd, then $M_{2m, m-k}(\{2\}) = 0$. Otherwise

$$M_{2m, m-k}(\{2\}) = \sum_{i=\max(0, \lceil \frac{m-3k}{2} \rceil)}^{\lfloor \frac{m-k}{2} \rfloor} C_{2k+i}^{m-k-i} \cdot C_{m-k-i}^i.$$

Then substituting $\lambda = \{3\}$ in (6), we get the required equality. $\square$

Remark 2. Equality (18) allows to calculate $\text{Hf}(T_{2m}(a, \{3\}, b))$ in polynomial time, at most in time $O(m^3)$.

Example 6. Consider the matrix $T_{2m}(0, \{3\}, 1)$. Calculating its hafnian by formula (18) for consecutive m 's, we get the sequence:

m	1	2	3	4	5	6	7	8	9	10	...
Hf	1	2	7	43	372	4027	51871	773186	13083385	247698481	...

Its m -th member equals the number of perfect matchings of the arc diagram $G_{2m}(0, \{2\}, 1)$ (Fig. 10). In other words, this is the number of linear chord diagrams with m chords such that the length of each chord does not equal 2 (the chord length in a linear chord diagram is determined in the same way as we determined the length of an arc in an arc diagram (see also [7])). This sequence has the number A265229 in [9], but its description does not contain the interpretation given here.

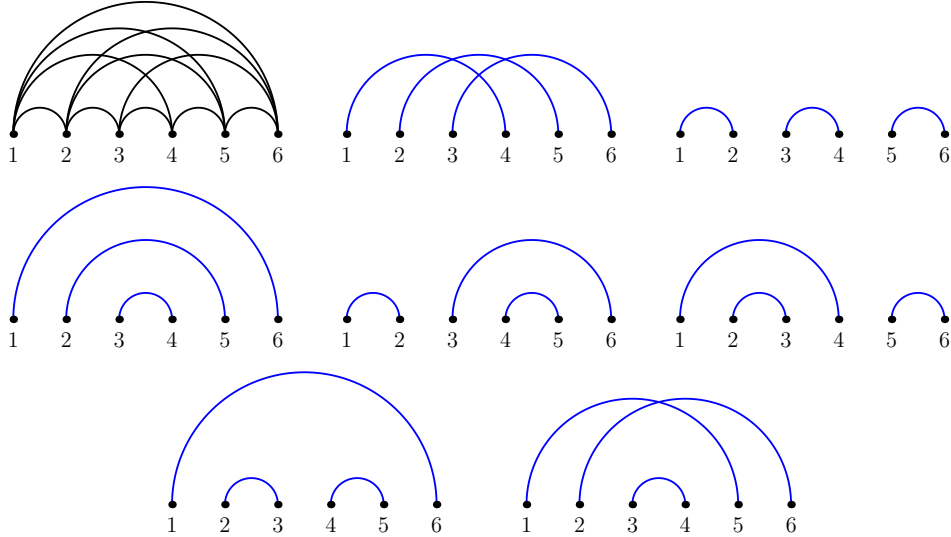


FIG. 10. The arc diagram $G_6(0, \{2\}, 1)$ and all its perfect matchings

6. CONCLUSION

We presented the general scheme for efficient exact computation of the hafnian of two-parameter Toeplitz matrices. This scheme is based on counting the number of matchings of λ -complete arc diagrams. In two special cases of $\{1\}$ -complete and $\{2\}$ -complete arc diagrams we give exact formulas. Based on these formulas, it

is not hard to write algorithms which calculate the hafnian of the corresponding matrices in polynomial time. The resulting formulas can be used to find the number of perfect matchings of special graphs, e.g. complements of the path graphs. Along the way, we established an interesting connection between the hafnian of Toeplitz matrices and the Bessel polynomials. This connection requires more detailed study. One could try, using the above methods, to find effective analytical formulas for calculating hafnians of other two-parameter Toeplitz matrices.

REFERENCES

- [1] E.R. Caianiello, *On quantum field theory - I: Explicit solution of Dyson's equation in electrodynamics without use of Feynman graphs*, IL Nuovo Cimento, **10**:12 (1953), 1634–1652.
- [2] A. Björklund, B. Gupt, N. Quesada, *A faster hafnian formula for complex matrices and its benchmarking on the Titan supercomputer*, arXiv:1805.12498v2, (2018).
- [3] G. Kuperberg, *Symmetries of plane partitions and the permanent-determinant method*, Journal of Combinatorial Theory, Series A, **68**:1 (1994), 115–151.
- [4] G. Kuperberg, *An exploration of the permanent-determinant method*, The Electronic Journal of Combinatorics, **5**, (1998), #R46.
- [5] M. Schwarz, *Efficiently computing the permanent and Hafnian of some banded Toeplitz matrices*, Linear Algebra and its Applications, **430**, (2009), 1364–1374.
- [6] E. Krasko, A. Omelchenko, *Enumeration of chord diagrams without loops and parallel chords*, Electronic Journal of Combinatorics, **24**:3, (2017), #3.43.
- [7] E. Sullivan, *Linear chord diagrams with long chords*, The Electronic Journal of Combinatorics, **24**:4, (2017), #4.20.
- [8] D.B. Efimov, *The hafnian and a commutative analogue of the Grassmann algebra*, Electronic Journal of Linear Algebra, **34**, (2018), 54–60.
- [9] N.J.A. Sloane, The On-Line Encyclopedia of Integer Sequences. Published electronically at <https://oeis.org/>, (2019).
- [10] H.L. Krall, O. Frink, *A new class of orthogonal polynomials: The Bessel polynomials*, Transactions of the American Mathematical Society, **65**, (1949), 100–115.
- [11] S.K. Chatterjea, *On the Bessel polynomials*, Rendiconti del Seminario Matematico della Università di Padova, **32**, (1962), 295–303.

DMITRY BORISOVICH EFIMOV
 INSTITUTE OF PHYSICS AND MATHEMATICS KOMI SCIENCE CENTRE URD RAS,
 KOMMUNISTICHESKAYA ST., 26,
 167000, SYKTYVKAR, RUSSIA
 E-mail address: dmefim@mail.ru